National Aeronautics and
Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

William Thigpen
NASA Advanced Supercomputing Division

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Resource Management System Version 1.4.8 Released

- HECC, in collaboration with NCCS, released version 1.4.8 of the Request Management System (RMS) on June 21, 2021. This tool replaced REI eBooks in March and is being updated to add features.
- Version 1.4.8 concentrates on multi-year requests and allocations, as well as preparing for the mission directorates' specific needs.
- The new RMS tool enables new features such as:
  - Easy navigation for requests from the home screen: Request more resources, Request more time, Cancel request, or Print PDF.
  - Allowing bulk allocation through Excel rather than allocating each individual allocation by hand.
  - Greater flexibility in customization and significant cost savings.
- On June 22, the new operational period (NOP) opened to all mission directorates on RMS.
- On June 28, an RMS user information session was held and was well-attended, with more than 55 participants.
- Completion of this milestone concluded the final phase of the multi-phase version 1.x project. Work on RMS 2.0, which will enhance administrative abilities, started immediately after the release.

IMPACT: Developing in-house software to manage supercomputer resource allocation requests allows NASA's High End Computing Program more ownership of the data and simplifies the process for reviewing allocations and targets.

Banner announcement of the Resource Management System version 1.4.8 release. *NASA*

Applications Team Updates Key Performance Benchmark

- HECC's Application Performance and Productivity (APP) team updated their version of the mesoscale weather benchmark: Weather Research and Forecasting (WRF) to version 3.9.1.1.
  - WRF is an important component of HECC's benchmark suite, which is heavily used to measure system health and performance.
  - It is also the best single representative of the entire SBU suite and is therefore used extensively for system architecture evaluations, including procurements.
- The previous WRF benchmark (v3.1) is more than 10 years old. The new version provides bug fixes, compatibility with more recent datasets, and backward compatibility with existing datasets.
  - Both WRF v3.9.1.1 and WRF v4.2.2 were evaluated against the Typhoon Morakot dataset in use since 2011.
  - WRF v3.9.1.1 was found to be more compatible with the dataset. Timings were found to fall within 5% of established wall times across architectures.
  - The APP team also improved validation testing by using the fldcor function from Climate Data Operators (CDO) to measure the correlation between sample variables.
- APP will continue evaluating WRFv4, which will likely involve the creation of a new test with a different dataset.

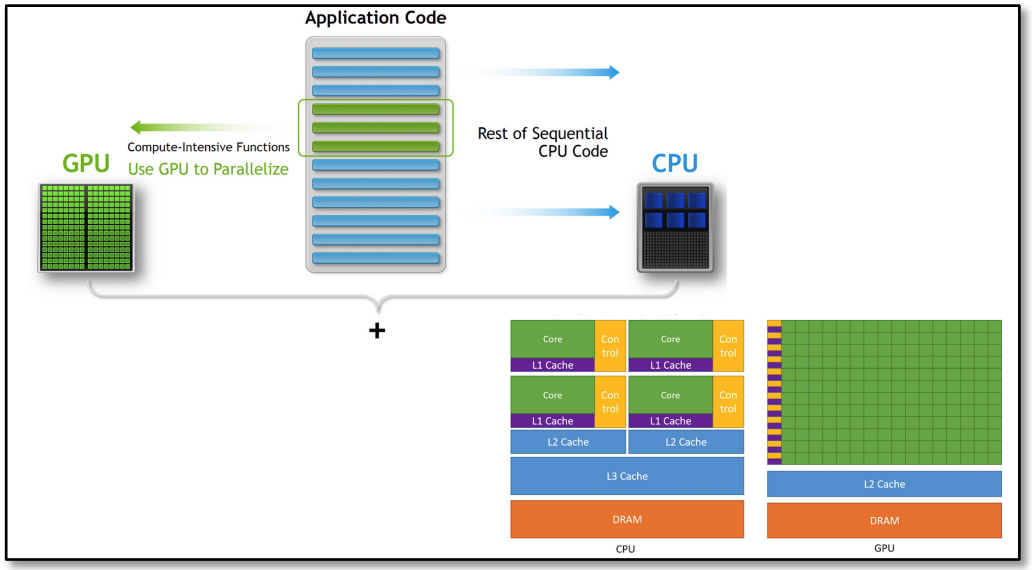
IMPACT: Benchmarks help maximize system productivity by identifying performance issues on existing systems and predicting the performance of architectures under consideration for acquisition.

HECC's Application Performance and Productivity team uses an established set of benchmarks to determine the health of existing systems, such as the Pleiades supercomputer (pictured above), and to predict the performance of potential new systems by comparing performance against reference statistics. *NASA/Ames*

HECC Contributes to Successful GPU Bootcamps

- HECC recently helped ensure the success of two virtual 6-hour GPU bootcamps organized by Eric Nielsen and George Switzer from Langley Research Center and staff from NVIDIA. The bootcamps are part of preparations for the NASA GPU Hackathon 2021, which is scheduled for September.
- More than 50 people attended the first event, which provided training on writing CUDA-enabled HPC applications to individuals with no prior GPU experience. More than 30 people attended the second event, which was tailored to artificial intelligence and machine learning applications. Many of the participants were new users who required NAS User Services assistance for account setup on short notice.
- HECC reserved 21 V100 GPU nodes for use by participants and provided technical support both before and during the events, including: devised and provided step-by-step instructions detailing the use of the Singularity container, Jupyter Lab, and SSH tunneling from users' local machines to the GPU nodes; tested NVIDIA's Singularity containers and prepared them for use by participants; and helped more than 20 participants by answering their questions and/or setting up their environments. Despite being given instructions to test logins and ssh tunneling in advance, many users waited until the time of the event to start setting up their accounts.
- Eric Nielsen was highly appreciative of the team's help. He wrote: "HUGE thanks to NAS for all of their support!"

IMPACT: Easing the process of porting legacy codes for use on accelerators will help ensure NASA's effective use of future high performance computing platforms.

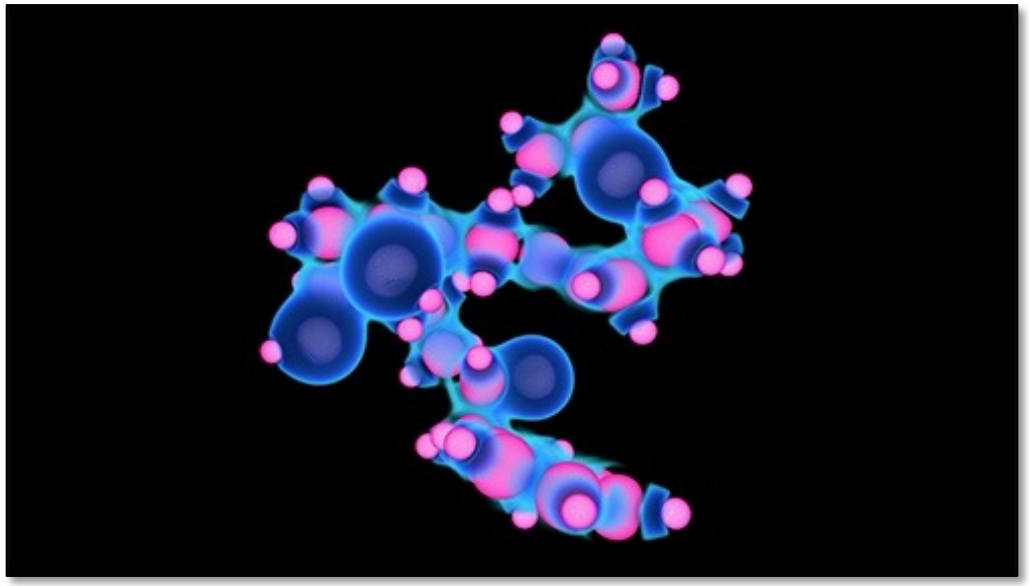


A chart included in one of the sessions of the first GPU bootcamp, highlighting the technique of splitting compute intensive functions and sequential code (top) and architectural differences (bottom) between graphics processing units and central processing units. *Image courtesy of NVIDIA.*

HECC Completes COVID-19 Consortium Research Projects

- As part of the COVID-19 High-Performance Computing Consortium, NASA provided access to HECC resources and expertise to support researchers in the fight to understand the pandemic and to develop treatments and vaccines.
- Three research projects completed their research utilizing their awarded supercomputing time on the HECC systems:
  - **MIT**: "Drug-repurposing for COVID-19 with 3D-aware Machine Learning." The models produced can accurately screen unknown compounds for SARS-CoV-2 inhibition. The work has led to 2 preprints, a publicly available dataset, and a publicly available code repository.
  - **NASA Ames**: "COVID-19 – RNA-seq Analysis to Identify Potential Biomarkers Indicative of Disease Severity." The researchers successfully analyzed 845 COVID-19 patient samples and environmental swab data to improve the understanding of SARS-CoV-2 interaction with the host. Results contributed to the collective scientific knowledge of COVID-19 through several publications, manuscripts-in-preparation, and presentations at scientific conferences including the 2020 supercomputing conference, SC20.
  - **Virginia Commonwealth University**: "Modeling the Dynamic Behavior of Surface Spike Glycoprotein of COVID19 Coronavirus and Designing Biomimetic Therapeutic Compounds." This work helped uncover dynamic and structural changes in spike protein variants that may lead to increased transmission rates. The project resulted in 2 publications.

IMPACT: HECC resources and services enabled COVID-19 scientists to conduct rapid research in the fight to stop the SARS-CoV-2 virus and find solutions that can help bring an end to the pandemic.

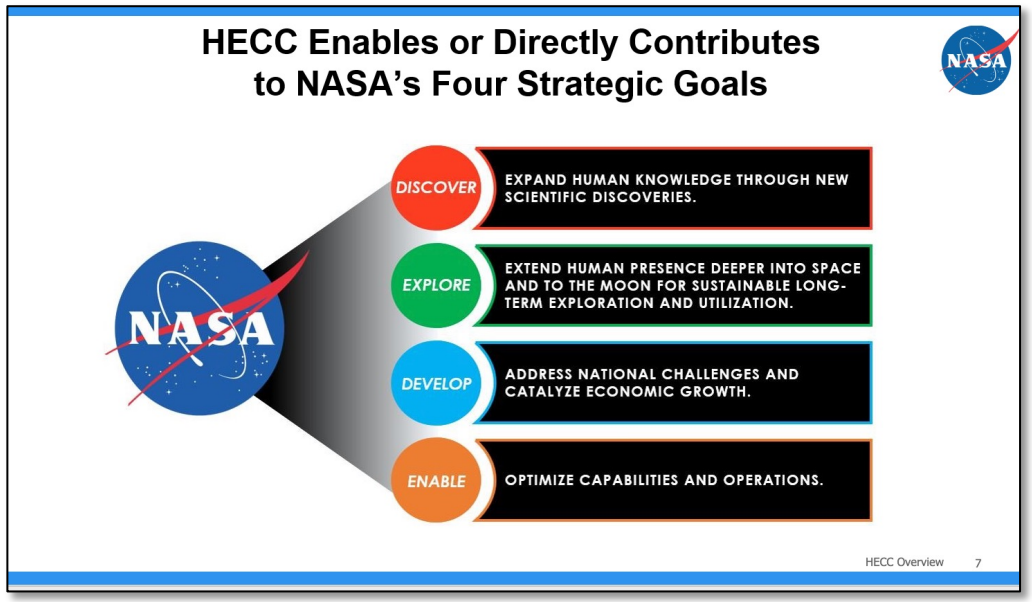


Simulation of the latanoprost molecule. A quantum chemistry calculation was performed at each step, yielding the energy, charge density, and atomic forces. Warm colors signify charge concentration and cool colors signify charge depletion. *Chris Henze, NASA/Ames*

HECC Support Teams Hold First Virtual User Meeting

- HECC completed the first of three virtual user meetings aimed at highlighting and promoting the project's extensive resources and services. Presentations covered the following support areas:
  - Overview of the HECC Project
  - User Services and Control Room
  - Cloud Offerings
  - Networks
  - Data Analytics/Publication/Discovery
  - Accounts and Allocations
  - Supercomputers/Filesystems
  - Application Optimization
  - Data Analysis/Visualization
  - Publications & Media
- These virtual meetings take the place of regular in-person outreach. Each meeting is targeted for a specific time zone (PDT, CDT, and EDT), to ensure the maximum number of participants.
  - The first meeting was very well attended, reaching 76 participants over the course of the session.
  - The remaining meetings will take place on July 7 and August 11.
- While not a perfect substitute for face-to-face meetings, this virtual component allows HECC to reach a much wider user base and will likely be used to supplement future outreach activities when regular travel resumes.

IMPACT: User outreach is critical to ensuring that scientists and engineers make the most of their compute resources and have an opportunity to give HECC staff a better understanding of their needs.



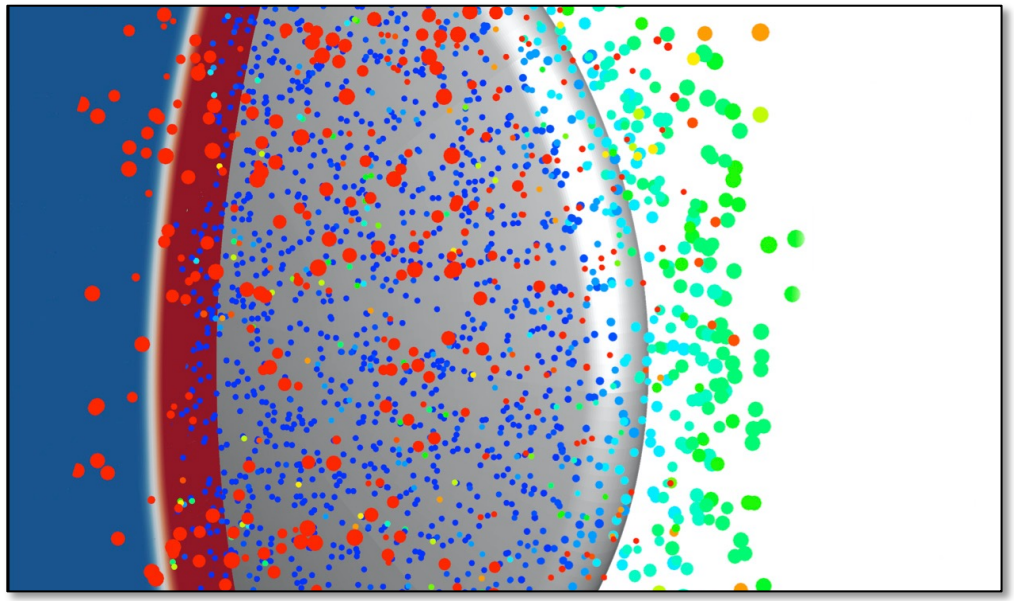
Slide from the HECC Overview presentation. All slides will be made available on the HECC website. *Bill Thigpen*

Modeling the Impact of Martian Dust on Entry Vehicles*

- The presence of suspended dust in the Martian atmosphere is a unique aspect of Mars atmospheric entry that current and future NASA missions to the Red Planet must address. Researchers from Stanford University used HECC resources to develop a computational methodology to efficiently and accurately simulate supersonic and hypersonic particle-laden flows over blunt bodies in order to better predict how entry vehicles will interact with the Martian atmosphere.
- The team used discontinuous Galerkin (DG) methods to perform simulations of hypersonic dusty flows and conducted a parametric study to address the lack of experimental data needed for validation.
- They also developed a Lagrangian particle method in the DG framework with algorithms to track particles on arbitrary elements, as well as to handle particle-fluid coupling and particle-particle interactions in an efficient and accurate manner.
- With this new methodology, the Stanford team found that their predictions of dust-induced surface heat flux augmentation agreed well with experimental tests, demonstrating the applicability of the computational models to accurately simulate the impact of suspended dust particles on thermal protection systems during atmospheric entry.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: Results of this work can be used to determine the types of test data needed from future experiments and guide the development of a simple, reliable physical model for use in the design of future missions to Mars.



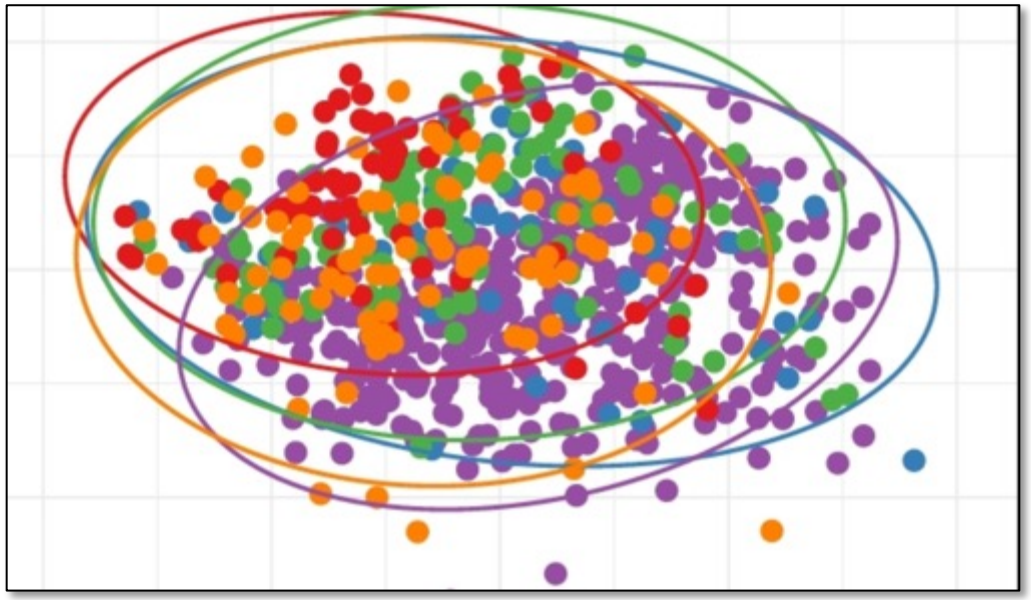
Visualization of a hypersonic dusty flow over a capsule forebody. The flow field is colored by the temperature of the gas (blue indicates low and red indicates high). The circles, which represent particles, are scaled in size by particle diameter and colored by streamwise velocity. *Eric Ching, Matthias Ihme, Stanford University*

Exploring the “Dark Genome” Response to SARS-CoV-2*

- A team of genetic researchers from NASA Ames, universities, and laboratories used Pleiades to perform transcriptomic (RNA) analysis of next-generation sequencing data from patients tested for SARS-CoV-2 to gain a better understanding of how the virus hijacks cells’ metabolic pathways to facilitate its own replication.
  - Human viruses may accomplish this by selectively modifying the host’s genomic output via interactions with genomic regulators such as non-coding RNA molecules (ncRNAs, also known as the “dark genome”).
- Results showed that SARS-CoV-2 infection induces a transcriptional shift—a shift in the genomic output—of the host cells, mainly characterized by an up-regulation of RNA transcripts that includes a specific group of long ncRNAs (lncRNAs).
  - The team postulated that lncRNAs appearing in higher amounts in patients infected with SARS-CoV-2—versus patients without SARS-CoV-2—will, in response to the infection, establish interaction networks with other cellular molecules such as RNA-binding proteins.
- Further characterization of these interactions may open a new window for the development of therapeutic strategies that could target lncRNA function in SARS-CoV-2 and other viral infections.

** HECC provided supercomputing resources and services in support of this work*

IMPACT: This work was part of the COVID-19 HPC Consortium, which provided high-performance computing access to researchers around the world studying the global transmission and impact of the COVID-19 virus.



Host transcriptomic analysis in SARS-CoV-2 infected samples. The chart shows Principal Component Analysis (PCA) of differentially expressed long non-coding RNAs (lncRNAs) in the infected samples. *Francisco J. Enguita, University of Lisbon, Portugal*

Papers

- "**Core Formation in High-z Massive Haloes: Heating by Post Compaction Satellites and Response to AGN Outflows**," A. Dekel, et al., arXiv:2106.01378 [astro-ph.GA], June 2, 2021. *
  https://arxiv.org/abs/2106.01378
- "**Molecular Dynamics Simulations of Ultrafast Radiation Induced Melting at Metal-Semiconductor Interfaces**," A. Ravichandran, et al., Journal of Applied Physics, vol .129, issue 21, published online June 2, 2021. *
  https://aip.scitation.org/doi/abs/10.1063/5.0045766
- "**One Year in the Life of Young Suns: Data Constrained Corona-Wind Model of kappa1 Ceti**," V. Airapetian, et al., arXiv:2106.01284 [astro-ph.SR], June 2, 2021. *
  https://arxiv.org/abs/2106.01284
- "**An Automated Bolide Detection Pipeline for GOES GLM**," J. Smith, R. Morris, C. Rumpf, R. Logenbaugh, N. McCurdy, C. Henze, J. Dotson, Icarus, vol. 368, June 4, 2021. *
  https://www.sciencedirect.com/science/article/pii/S0019103521002451
- "**The Interaction Between Rising Bubbles and Cold Fronts in Cool Core Clusters**," A. C. Fabian, J. Zuhone, S. A. Walker, arXiv:2106.03663 [astro-ph.GA], June 7, 2021. *
  https://arxiv.org/abs/2106.03662
- "**Planet Hunters TESS III: Two Transiting Planets around the Bright G Dwarf HD 1528443**," N. Eisner, et al., arXiv:2106.04603 [astro-ph.EP], June 8, 2021. *
  https://arxiv.org/abs/2106.04603

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Dynamical Effects of Cosmic Rays on the Medium Surrounding Their Sources**," B. Schroer, et al., The Astrophysical Journal Letters, vol. 914, no. 1, June 9, 2021. *
  https://iopscience.iop.org/article/10.3847/2041-8213/ac02cd/meta
- "**From Electrons to Janskys: Full Stokes Polarized Radiative Transfer in 3D Relativistic Particle-in-Cell Jet Simulations**," N. MacDonald, K.-I. Nishikawa, arXiv:2106.04915 [astro-ph.HE], June 9, 2021. *
  https://arxiv.org/abs/2106.04915
- "**A Perspective on Collective Properties of Atoms on 2D Materials**," A. Del Maestro, et al., arXiv:210.07685 [cond-mat.mes-hall], June 14, 2021. *
  https://arxiv.org/abs/2106.07685
- "**Lepton-Driven Non-Resonant Streaming Instability**," S. Gupta, et al., arXiv:2106.07672 [astro-ph.HE], June 14, 2021. *
  https://arxiv.org/abs/2106.07672
- "**TESS Data for Astroseismology: Photometry**," R. Handberg, et al., arXiv:2106.08341 [astro-ph.IM], June 15, 2021. *
  https://arxiv.org/abs/2106.08341
- "**Atomic-Scale Evidence for Open-System Thermodynamics in the Early Solar Nebula**," T. Zega, et al., The Planetary Science Journal, vol. 2, no. 3, June 17, 2021. *
  https://iopscience.iop.org/article/10.3847/PSJ/abf5e5/meta

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Efficiency of Mixed-Element USM3D for Benchmark Three-Dimensional Flows**," M. Pandya, D. Jespersen, B. Diskin, J. Thomas, N. Frink, AIAA Journal, published online June 21, 2021. *
  https://arc.aiaa.org/doi/full/10.2514/1.J059720

** HECC provided supercomputing resources and services in support of this work*

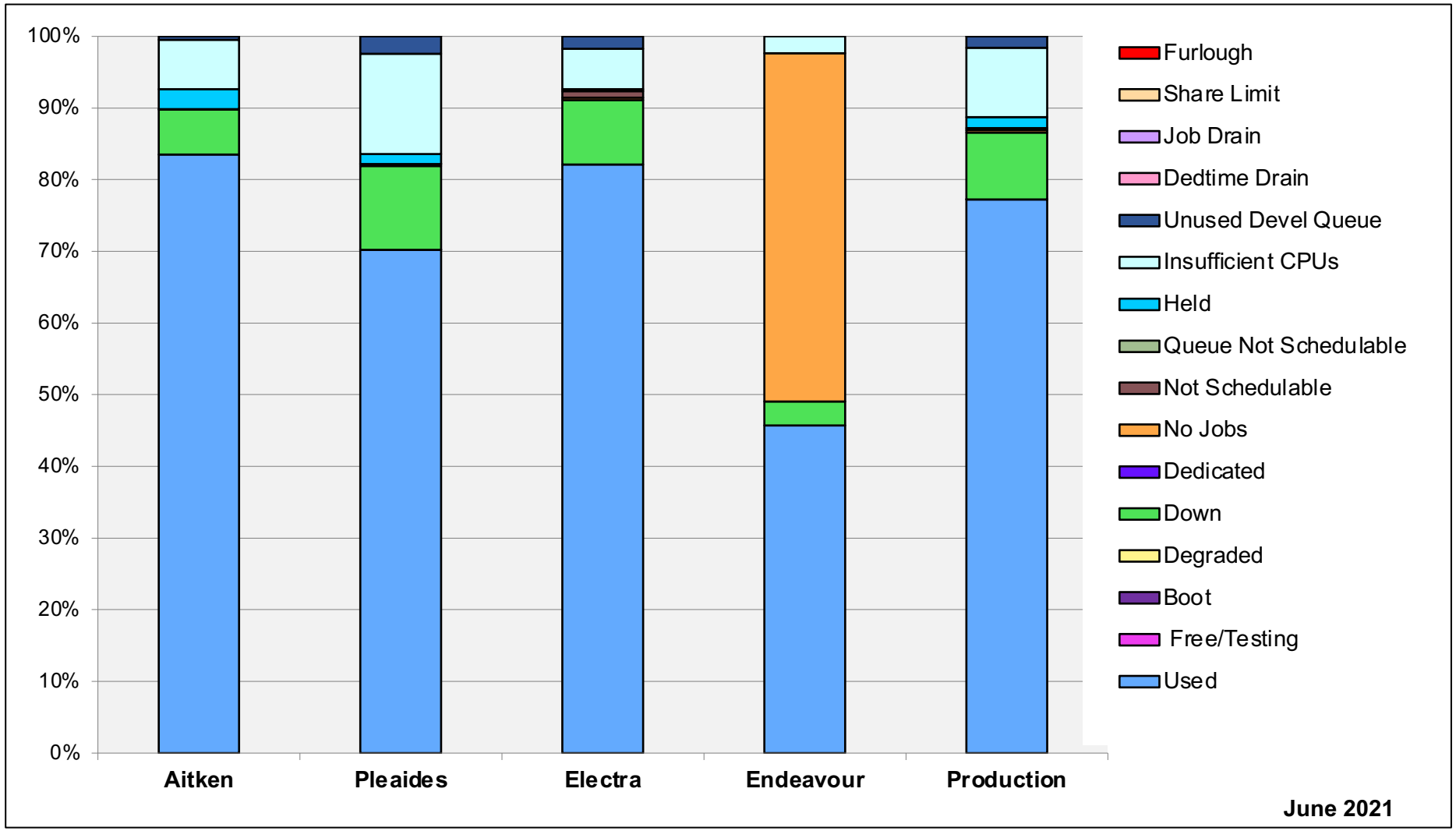
News and Events

- **Which Way Does the Solar Wind Blow?** *Texas Advanced Computing Center*, June 3, 2021—Using supercomputers at NAS, as well as the Texas Advanced Computing Center and the San Diego Supercomputing Center, researchers are improving models and methods to predict space weather, including the arrival of coronal mass ejections.
  https://www.tacc.utexas.edu/-/which-way-does-the-solar-wind-blow-
  - **Which Way Does the Solar Wind Blow? Supercomputers Improve Space Weather Prediction**, *SciTech Daily*, June 6, 2021.
    https://scitechdaily.com/which-way-does-the-solar-wind-blow-supercomputers-improve-space-weather-prediction/
  - **Space Weather Prediction Gets a Supercomputing Boost**, *HPCwire*, June 9, 2021.
    https://www.hpcwire.com/2021/06/09/space-weather-prediction-gets-a-supercomputing-boost/
  - **UAH-Led Space Weather Prediction Research Could be Critical to U.S. Space Command**, *University of Alabama in Huntsville*, June 24, 2021.
    https://www.uah.edu/news/items/uah-led-space-weather-prediction-research-could-be-critical-to-space-force-command
- **NASA Partners with Khaled bin Sultan Living Oceans Foundation to Expand Efforts to Map Corals**, *NASA Ames*, June 8, 2021—NASA's Ames Research Center is partnering with the Khaled bin Sultan Living Oceans Foundation to use their extensive high-resolution data about reefs and expand NASA's coral mapping capabilities even further. The partnership will use the massive Global Reef Expedition dataset in conjunction with the neural network and the Pleiades supercomputer at the NAS facility.
  https://www.nasa.gov/image-feature/ames/nasa-expands-efforts-to-map-corals
  - **Mapping the World's Coral Reefs**, *World Ocean Forum*, June 8, 2021.
    https://medium.com/world-ocean-forum/mapping-of-the-worlds-coral-reefs-e29ba653a049

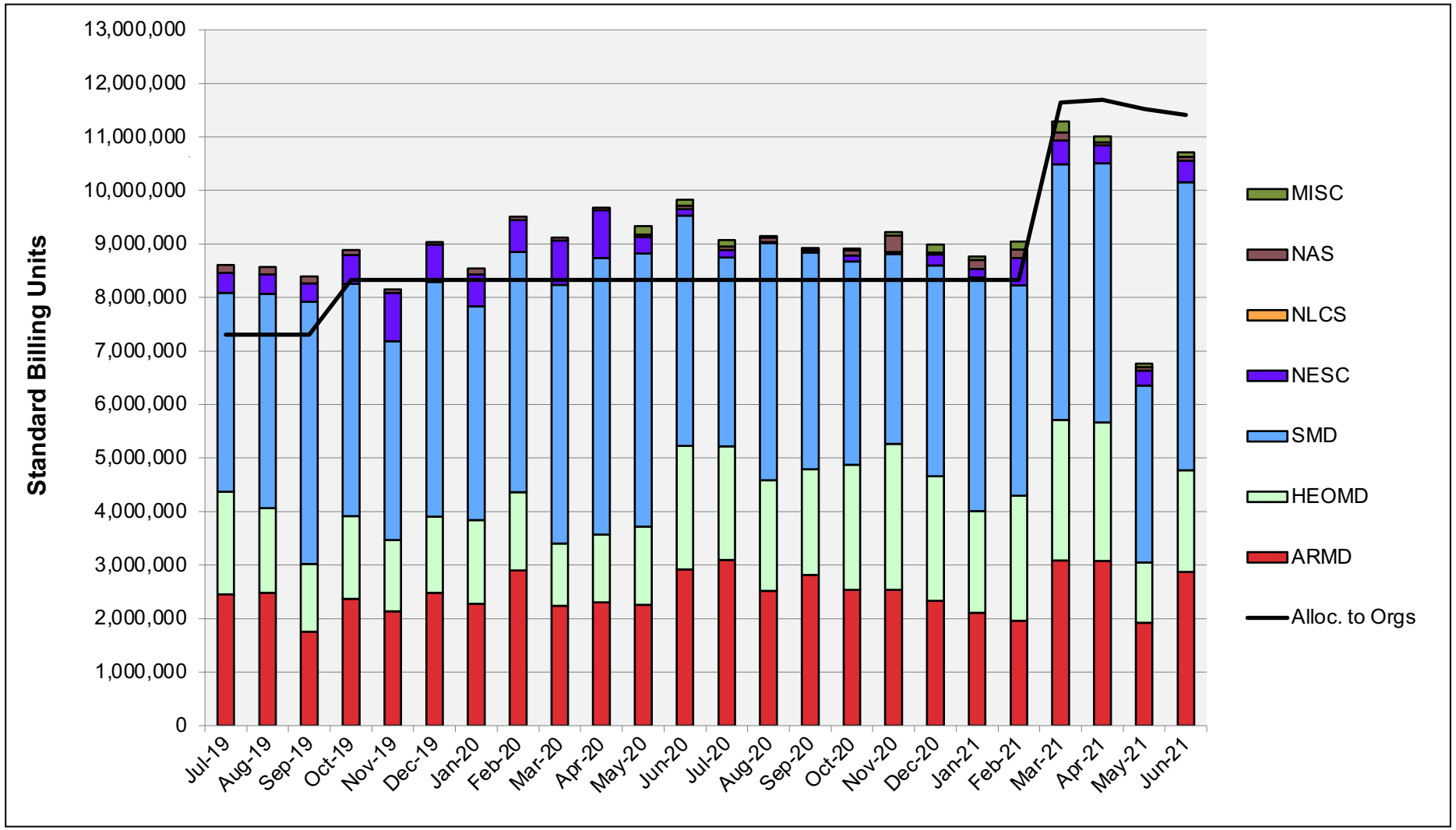
News and Events: Social Media

- **Coverage of NAS Stories**
  - Aitken compute hours milestone:
    - NAS: Twitter 2 retweets, 6 favorites.
    - NASA Supercomputing: Facebook 639 users reached, 101 engagements, 7 likes, 4 shares.
  - NAS Software Available to Public (part of NASA's updated software catalog campaign):
    - NAS: Twitter 5 retweets, 31 favorites.
    - NASA Supercomputing: Twitter 3 retweets, 7 favorites; Facebook 236 users reached, 8 engagements, 4 likes.
  - Asteroid Threat Assessment Project (Asteroid Day):
    - NASA Ames: Twitter 28 retweets, 102 favorites; Facebook 40 likes, 17 comments, 15 shares.
    - NASA Supercomputing: Facebook 62 users reached, 11 engagements, 5 likes.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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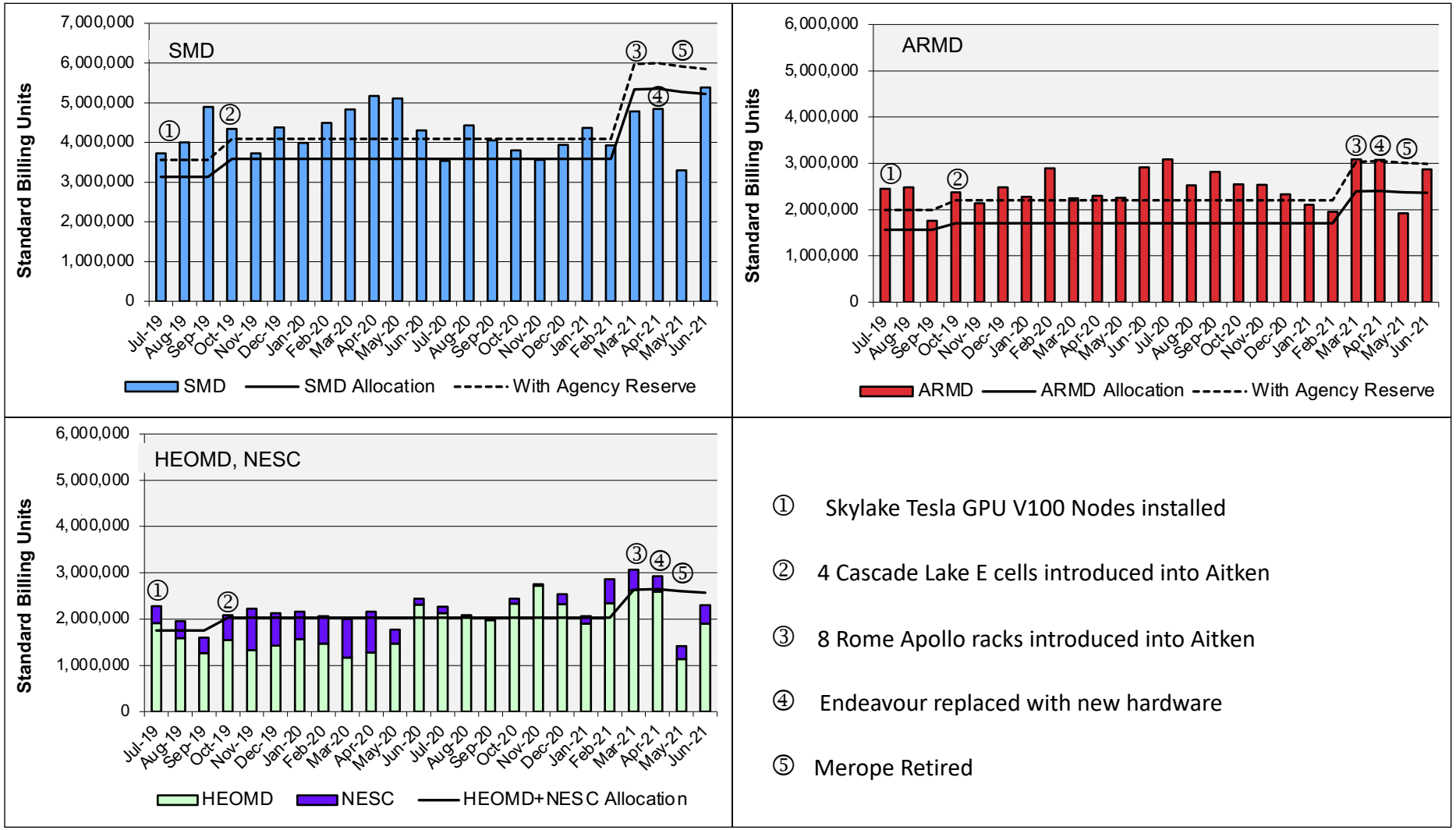


① Skylake Tesla GPU V100 Nodes installed

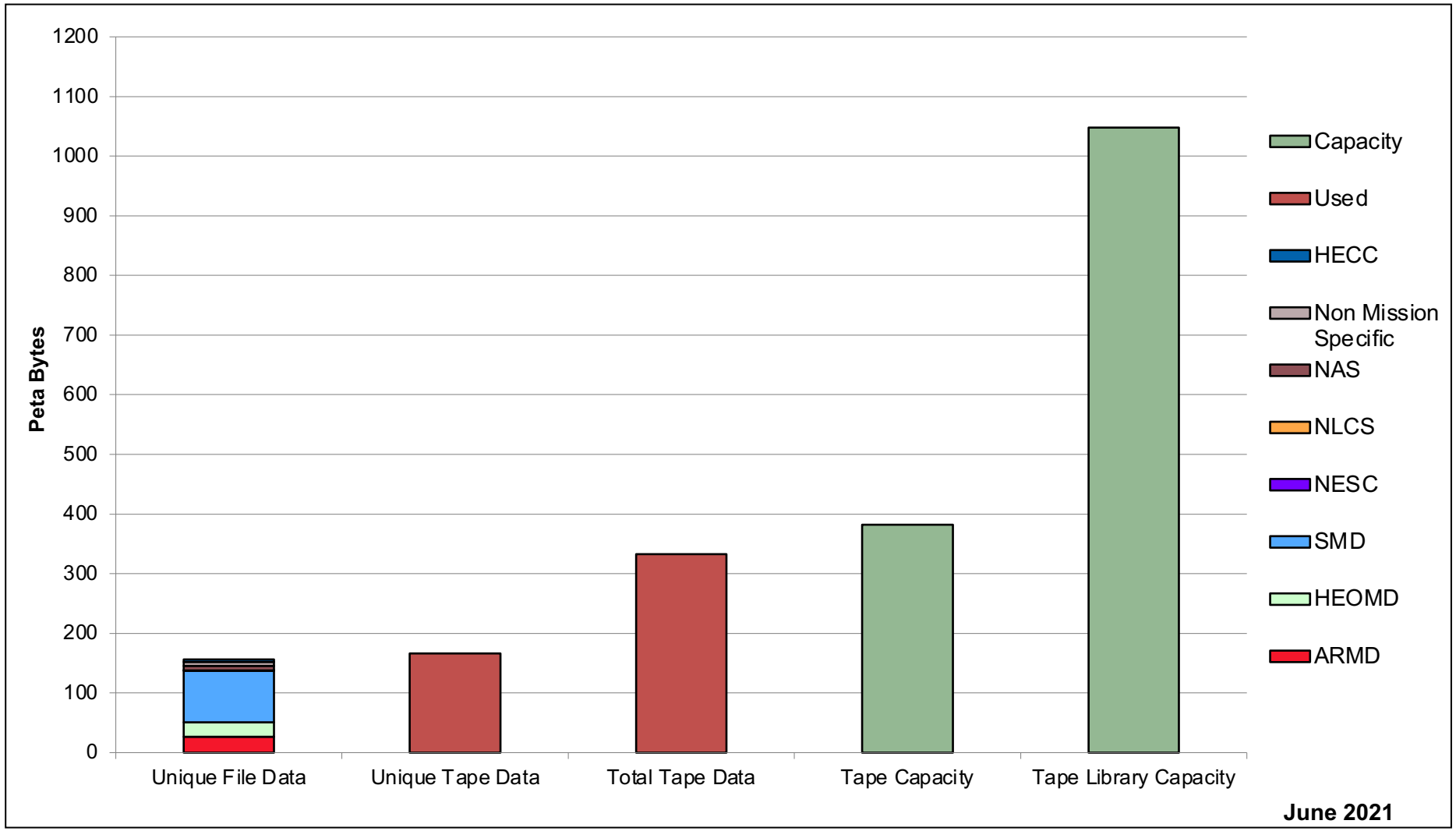
② 4 Cascade Lake E cells introduced into Aitken

③ 8 Rome Apollo racks introduced into Aitken

④ Endeavour replaced with new hardware

⑤ Merope Retired

Tape Archive Status



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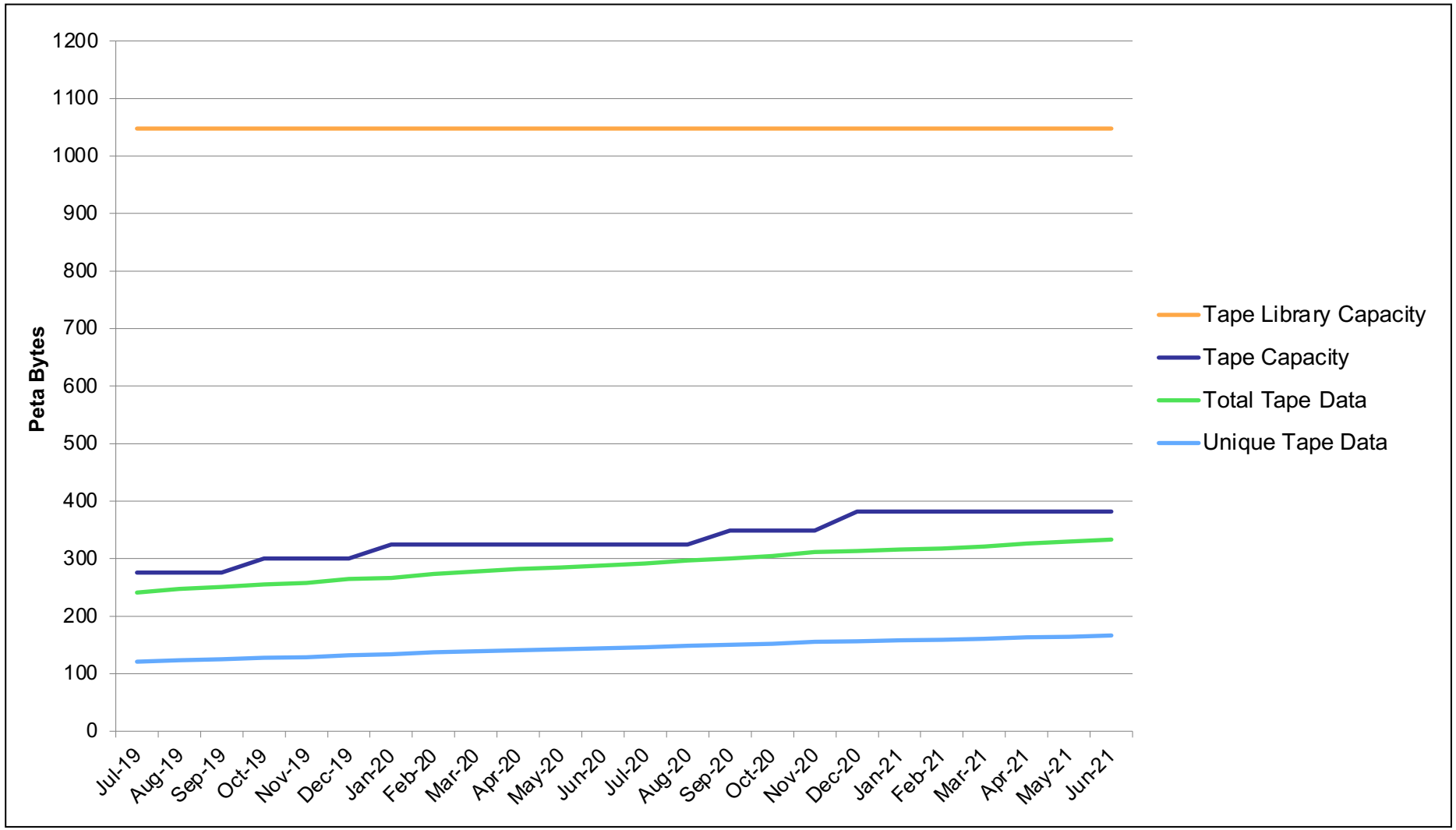
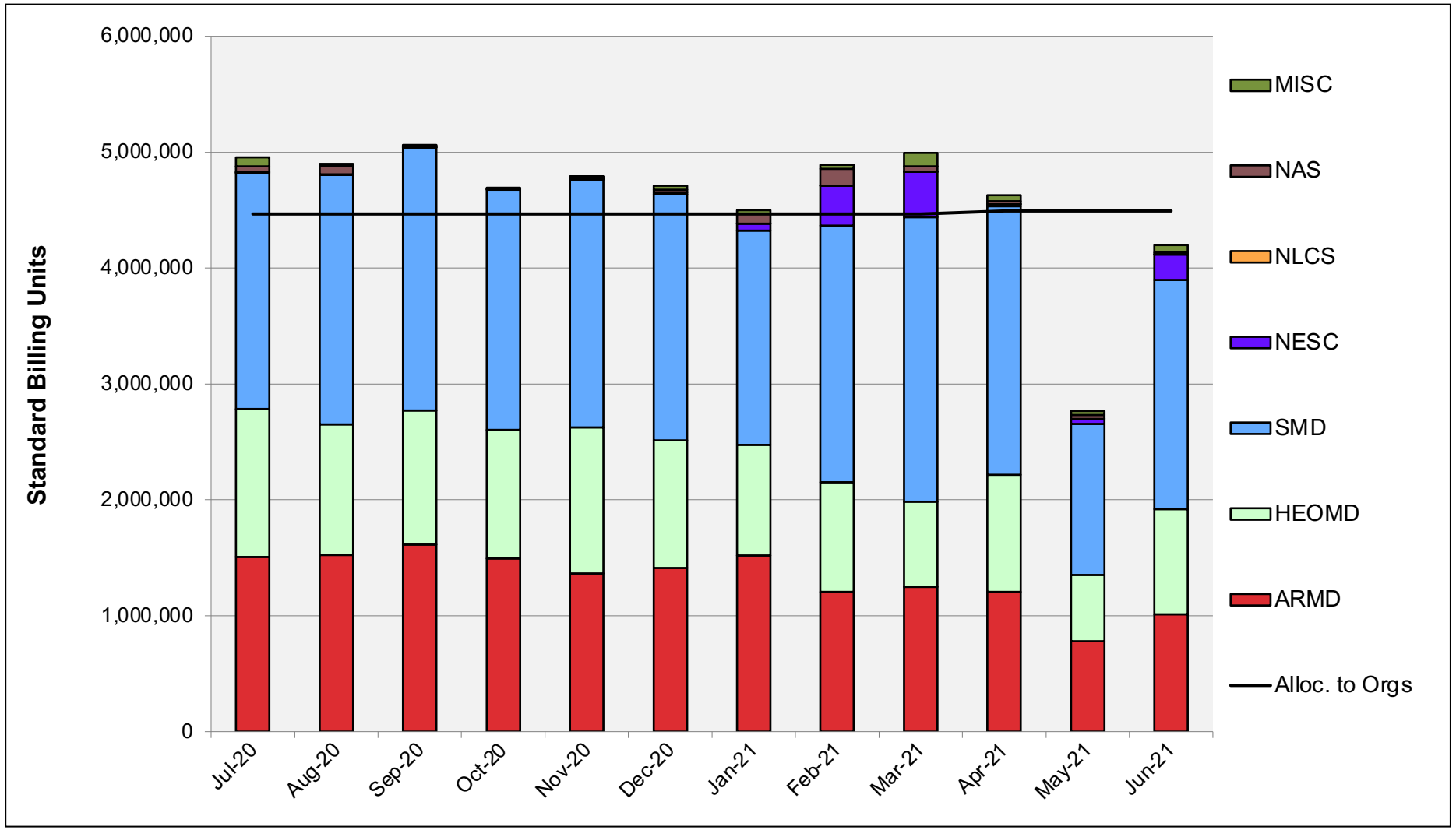
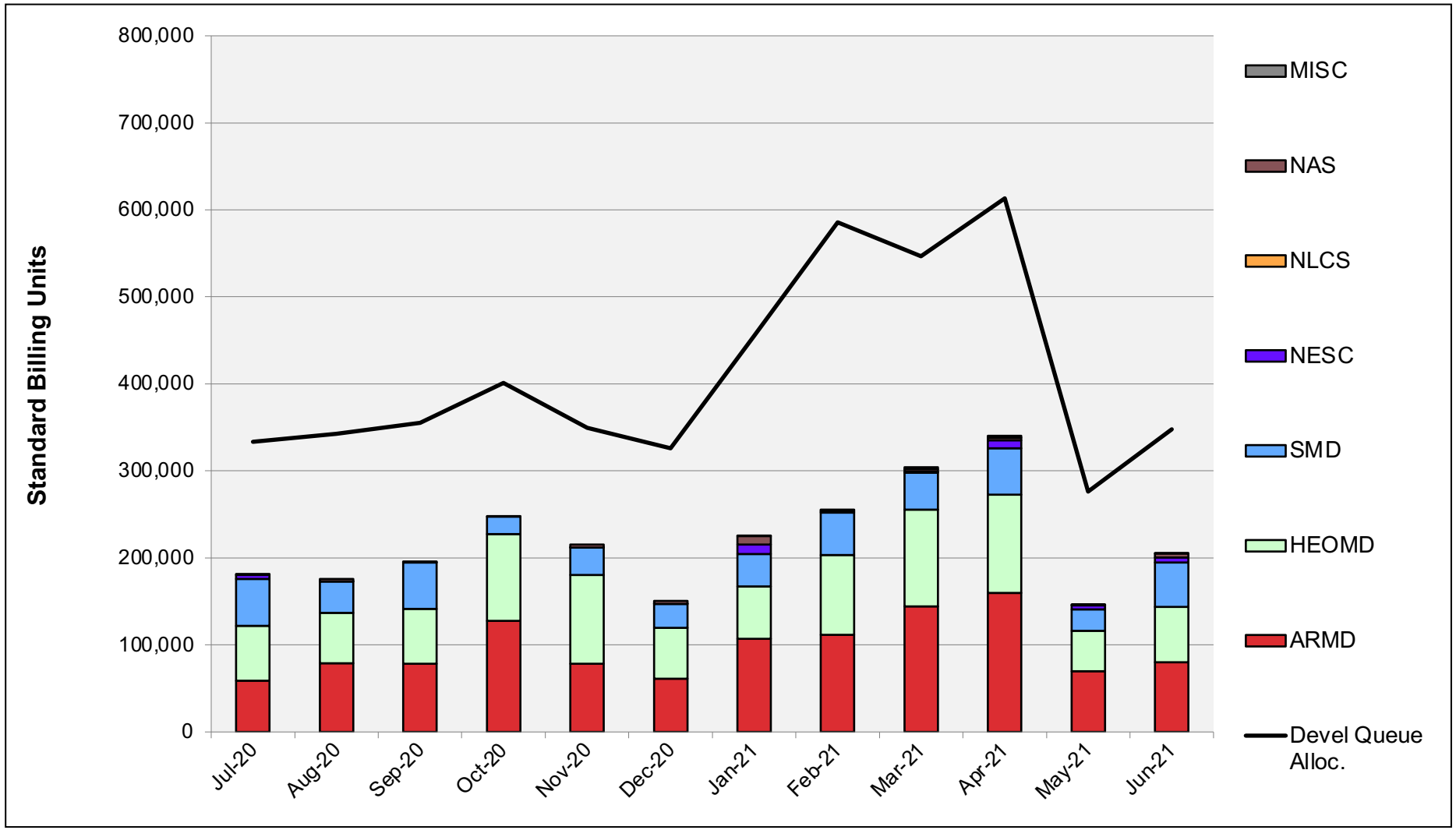


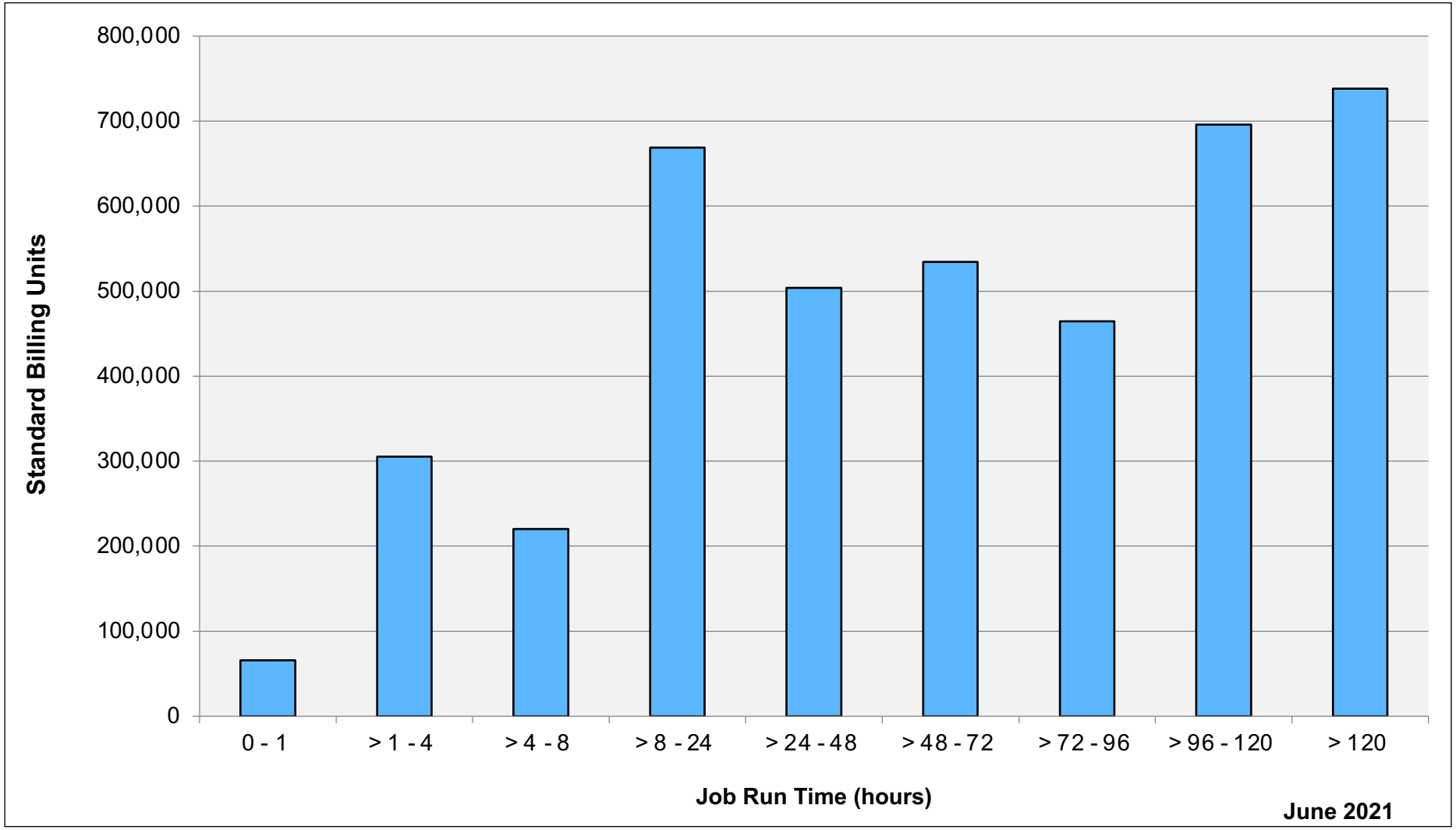
Pleiades: SBUs Reported, Normalized to 30-Day Month



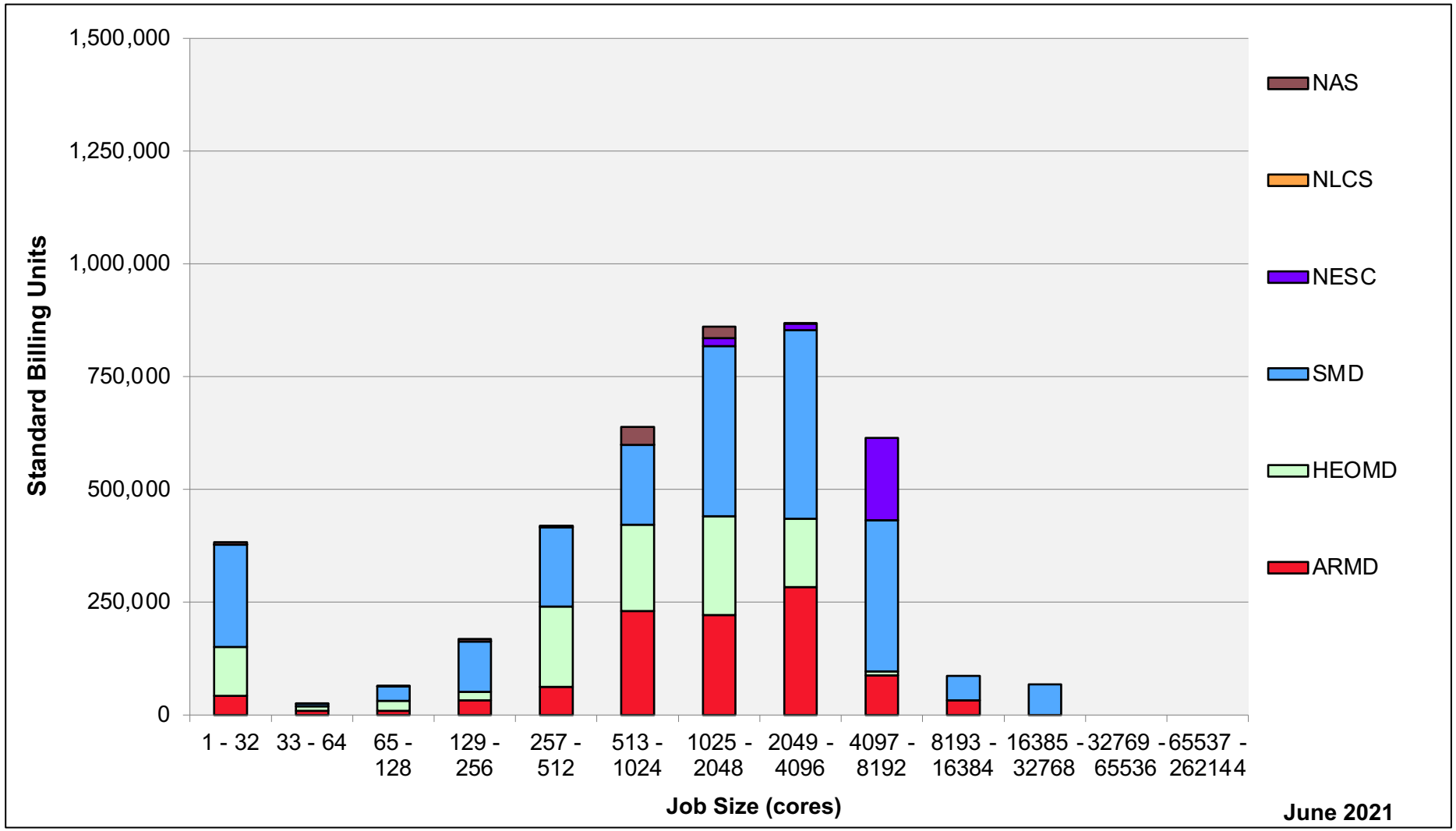
Pleiades: Devel Queue Utilization



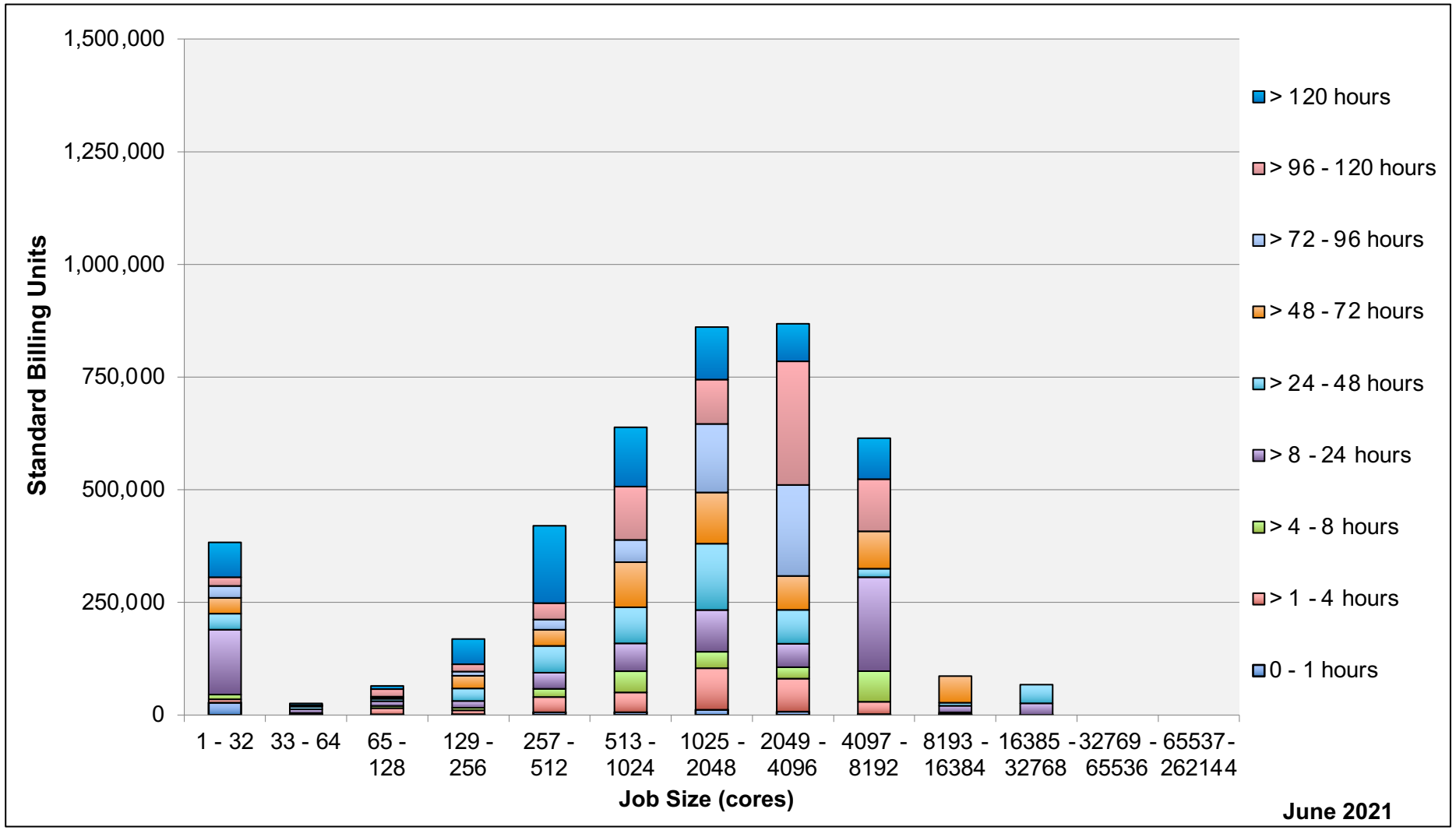
Pleiades: Monthly Utilization by Job Length



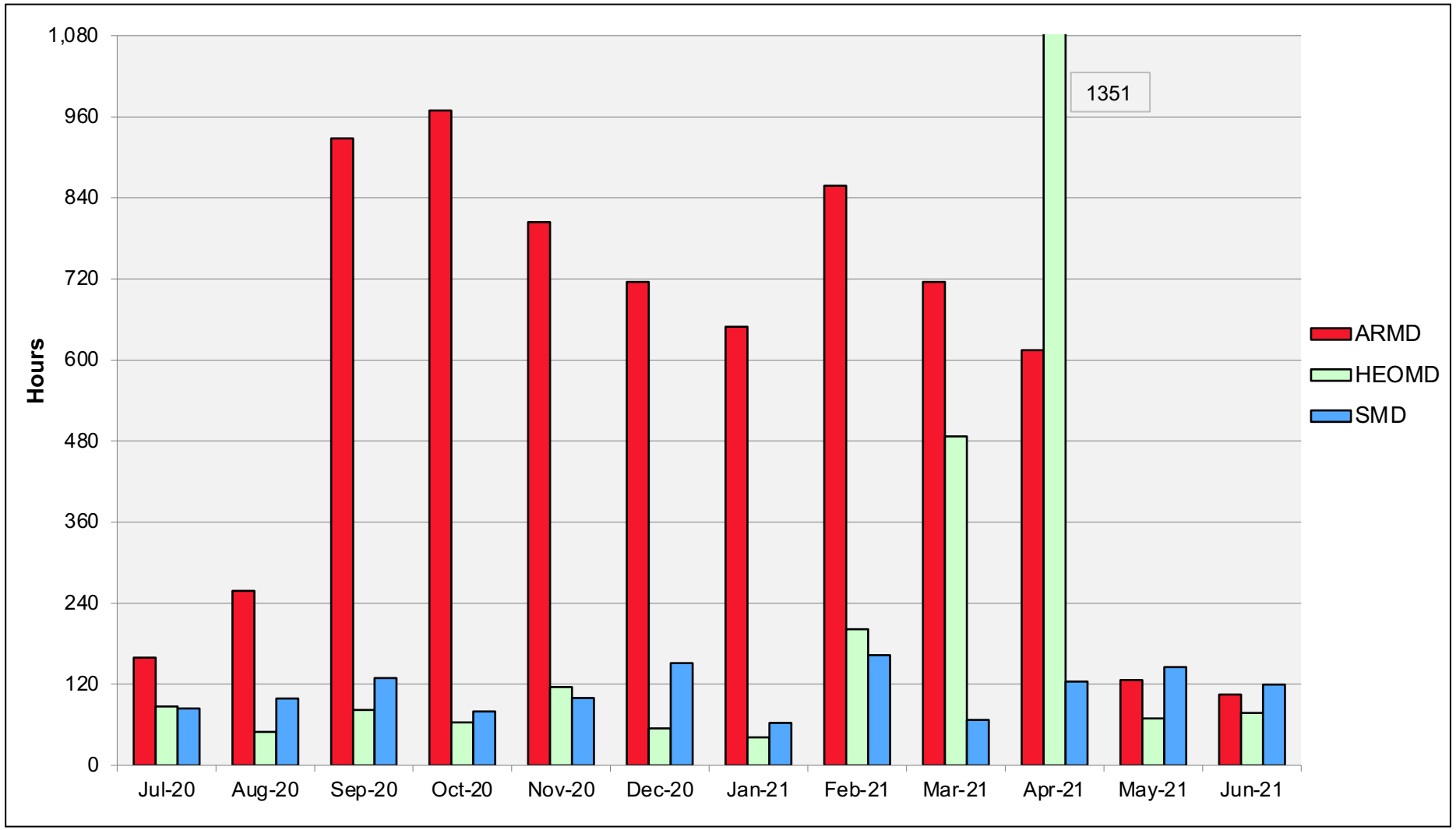
Pleiades: Monthly Utilization by Job Size



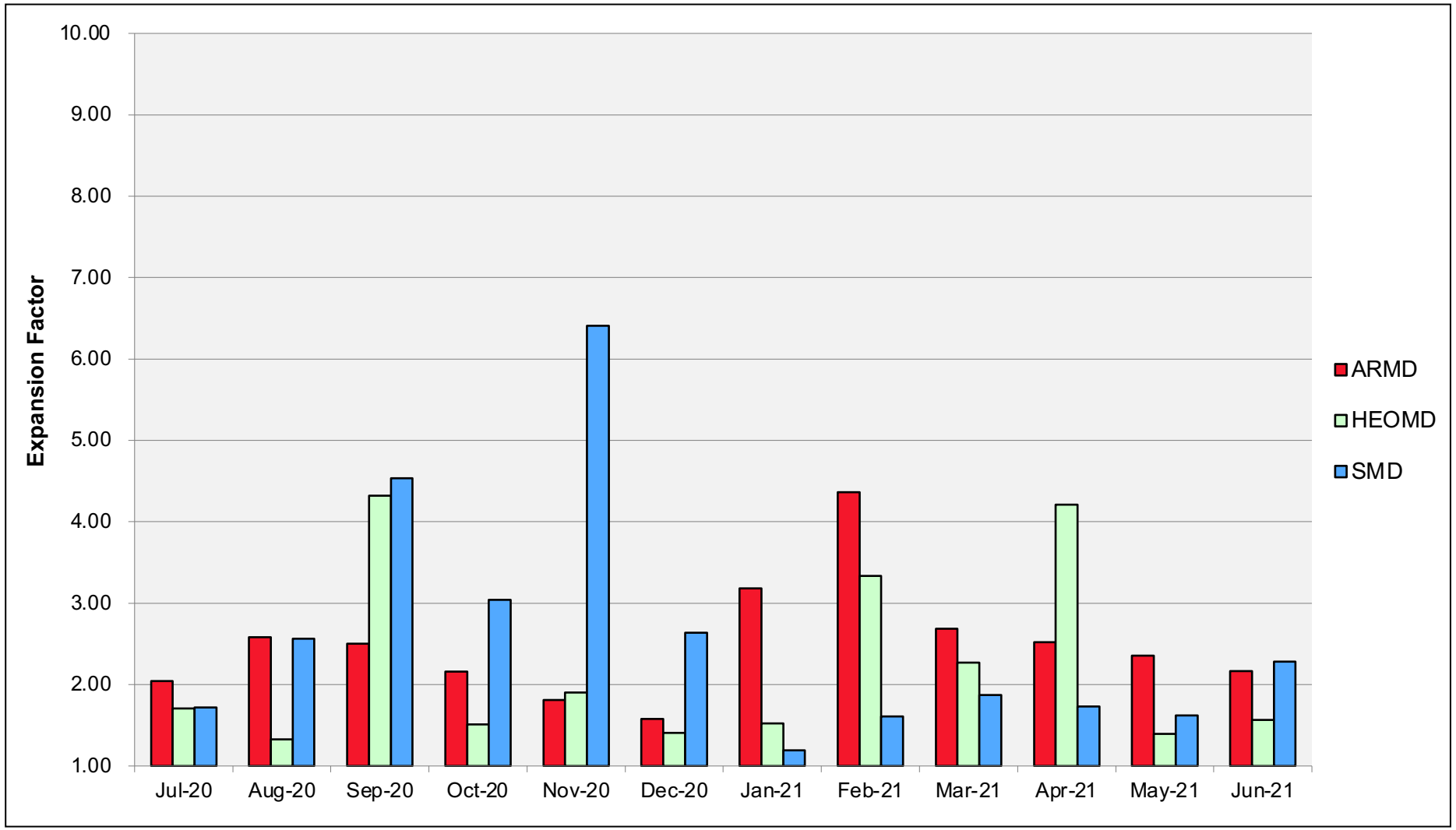
Pleiades: Monthly Utilization by Size and Length



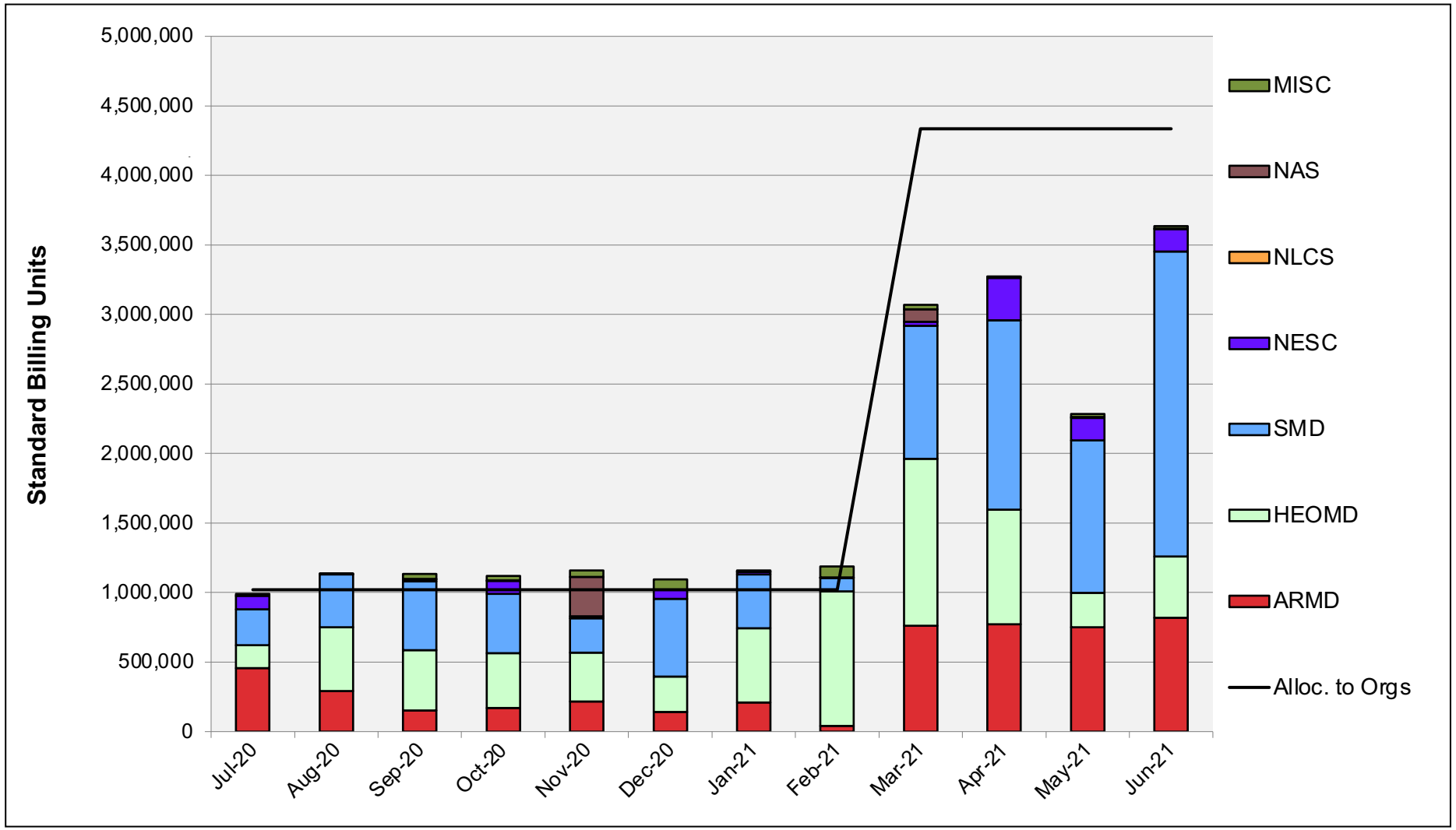
Pleiades: Average Time to Clear All Jobs



Pleiades: Average Expansion Factor



Aitken: SBUs Reported, Normalized to 30-Day Month



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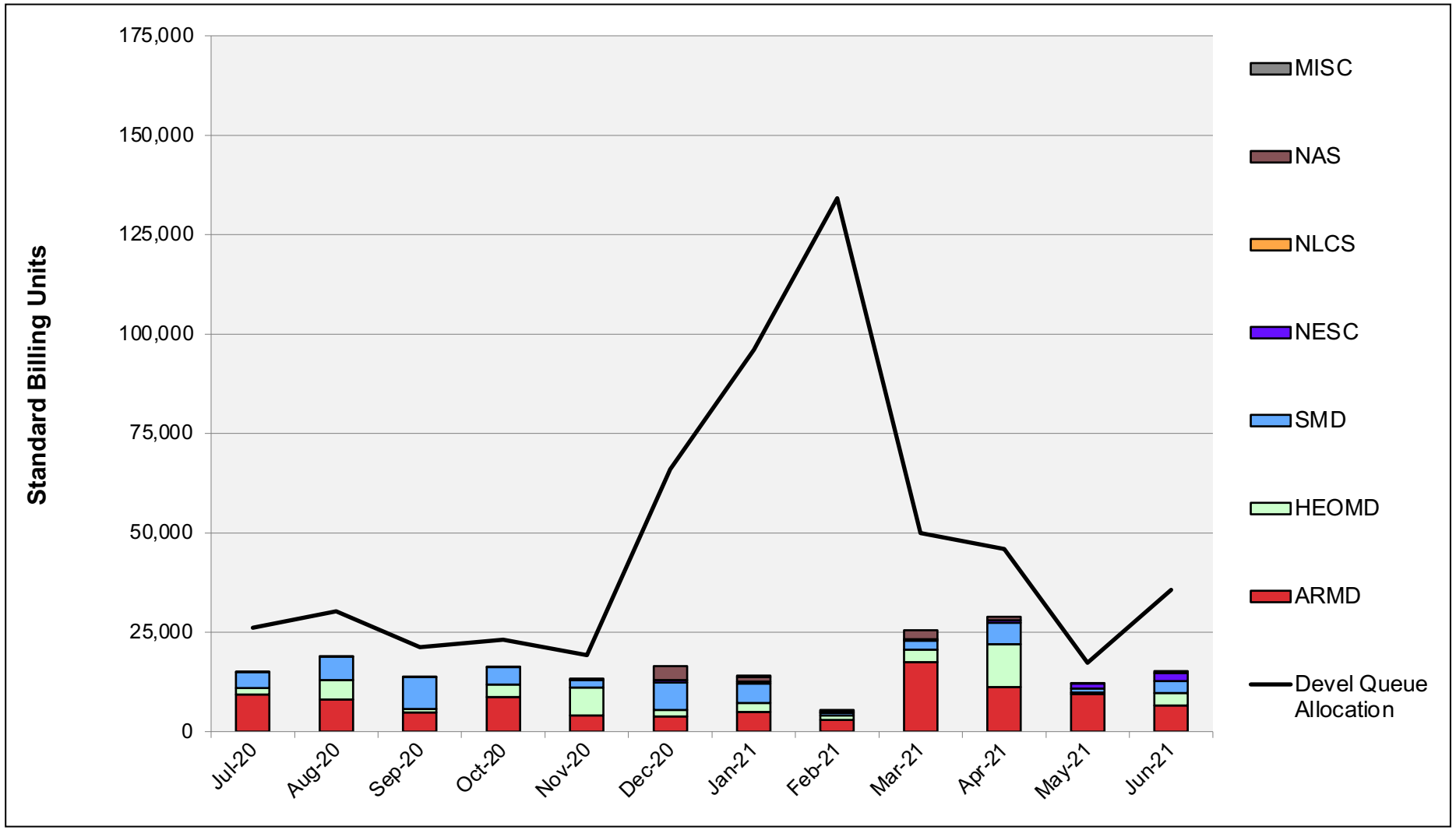

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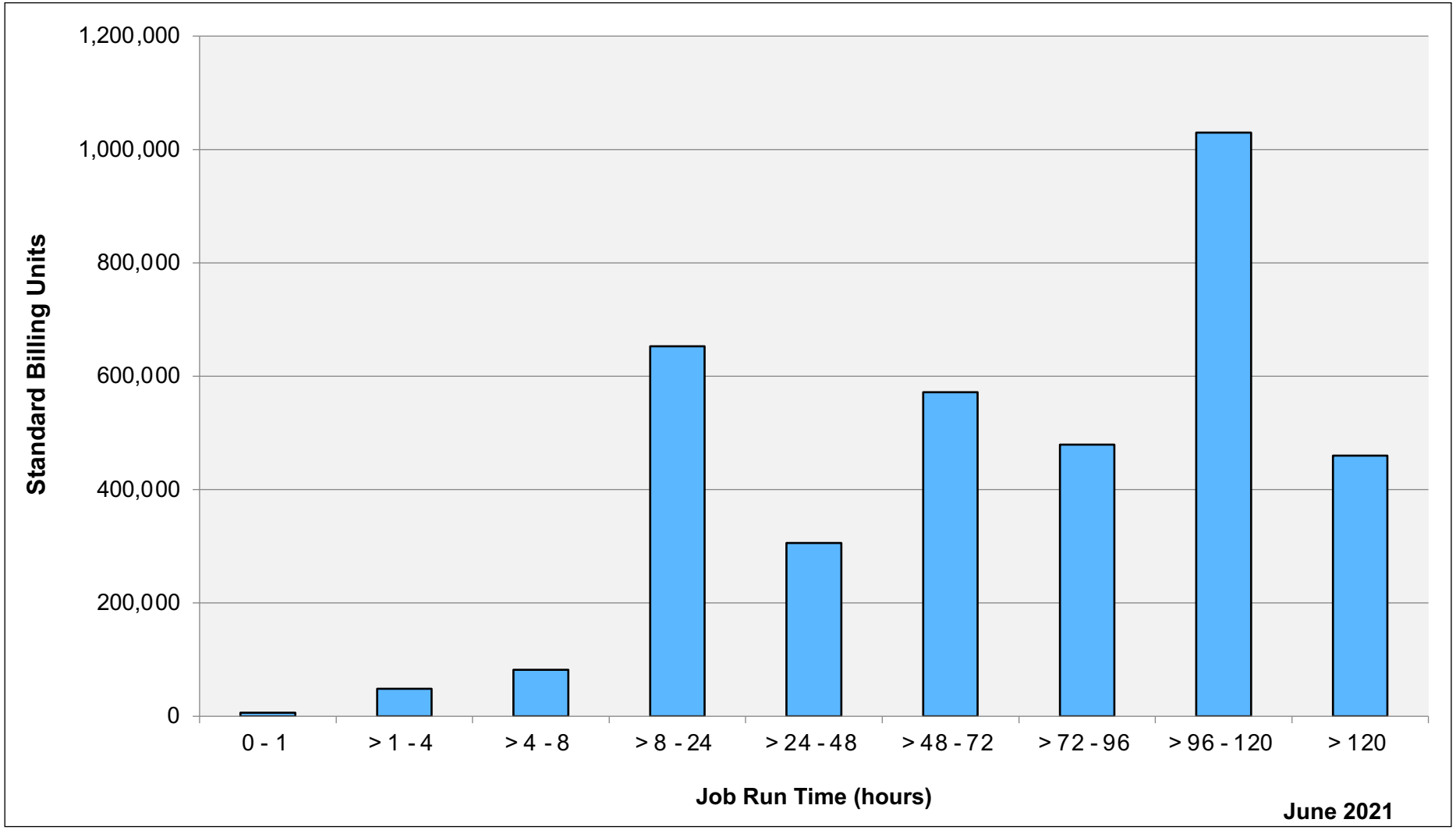

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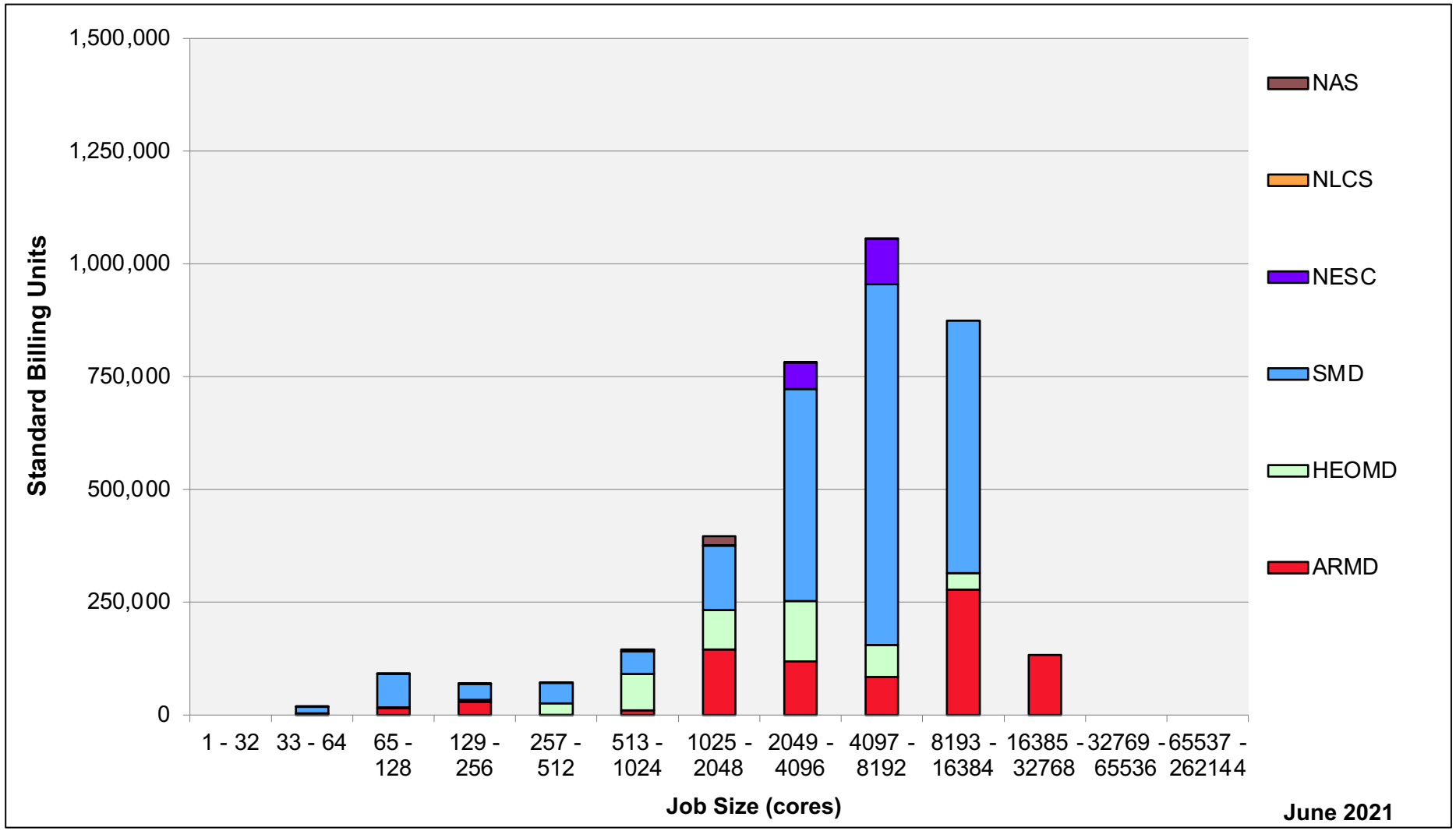
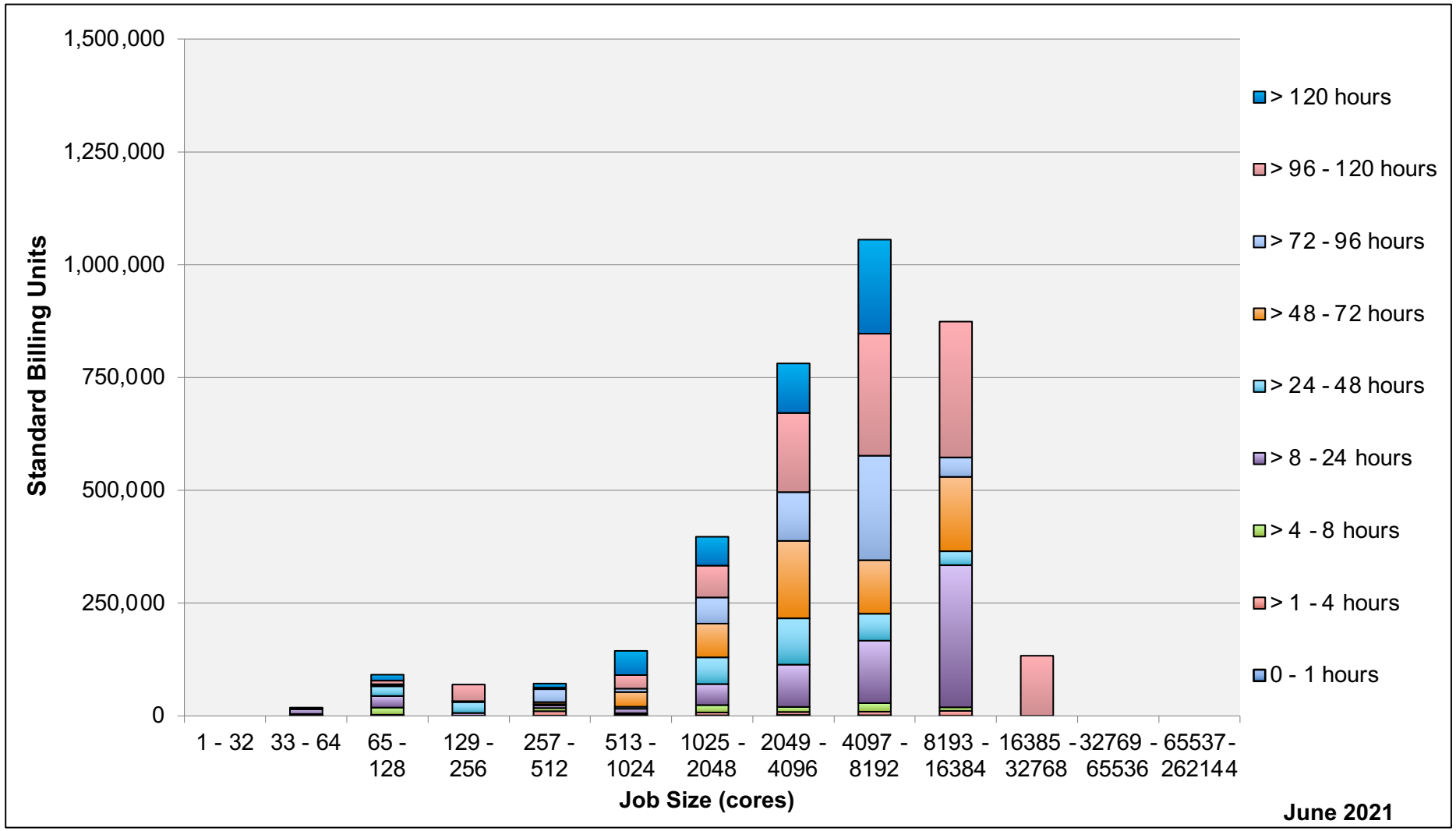


Aitken: Monthly Utilization by Size and Length



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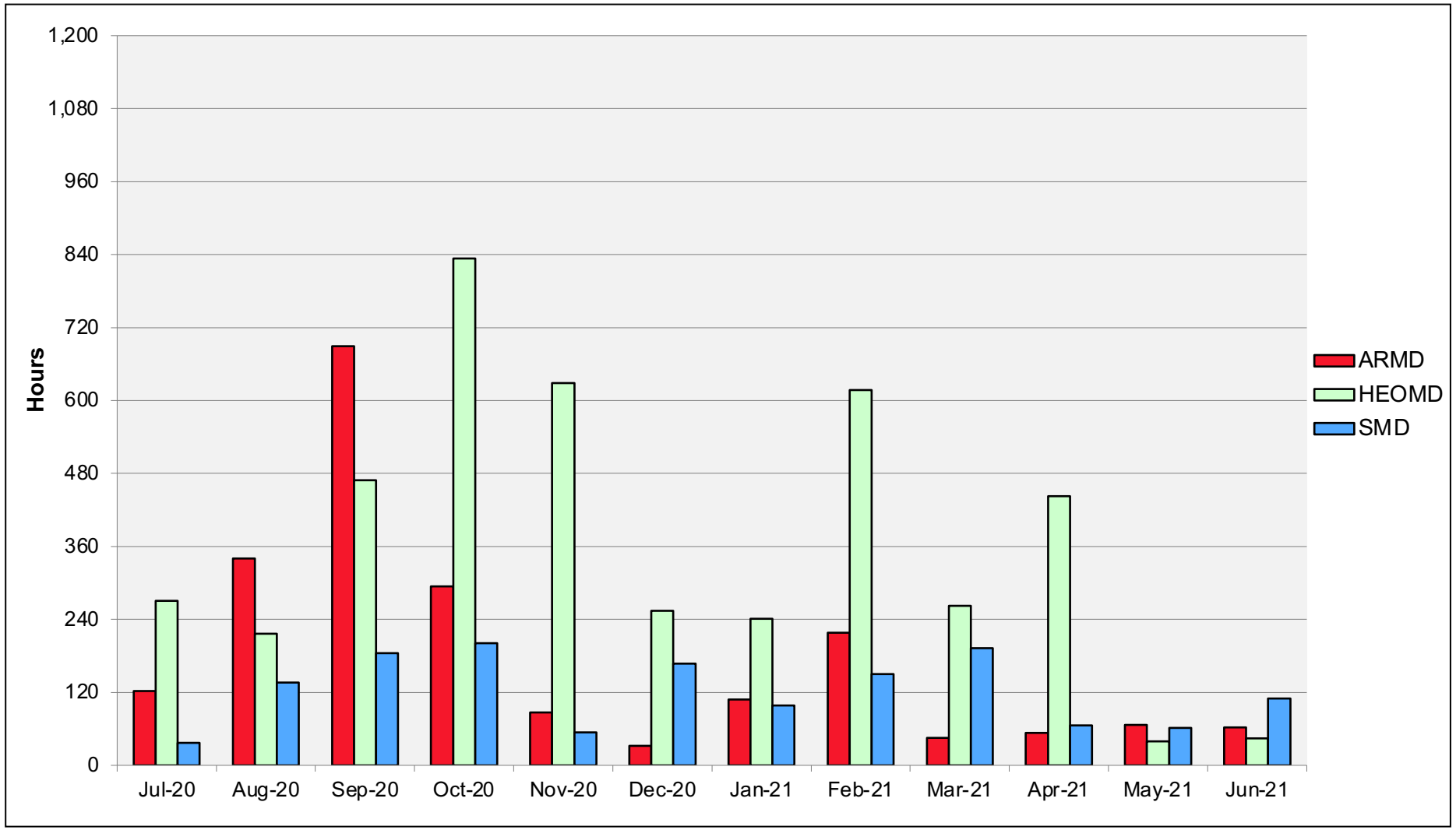
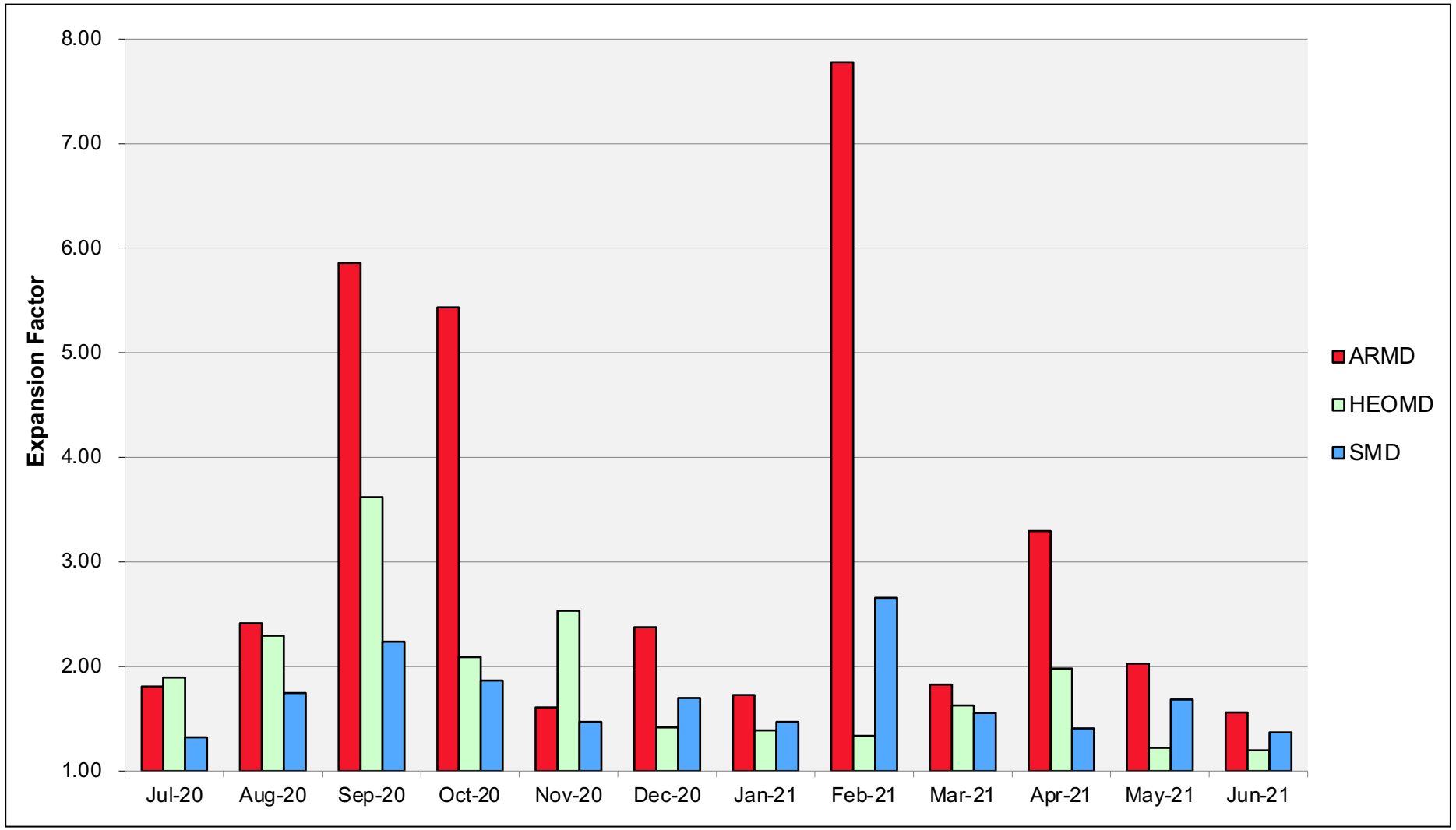


Aitken: Average Expansion Factor



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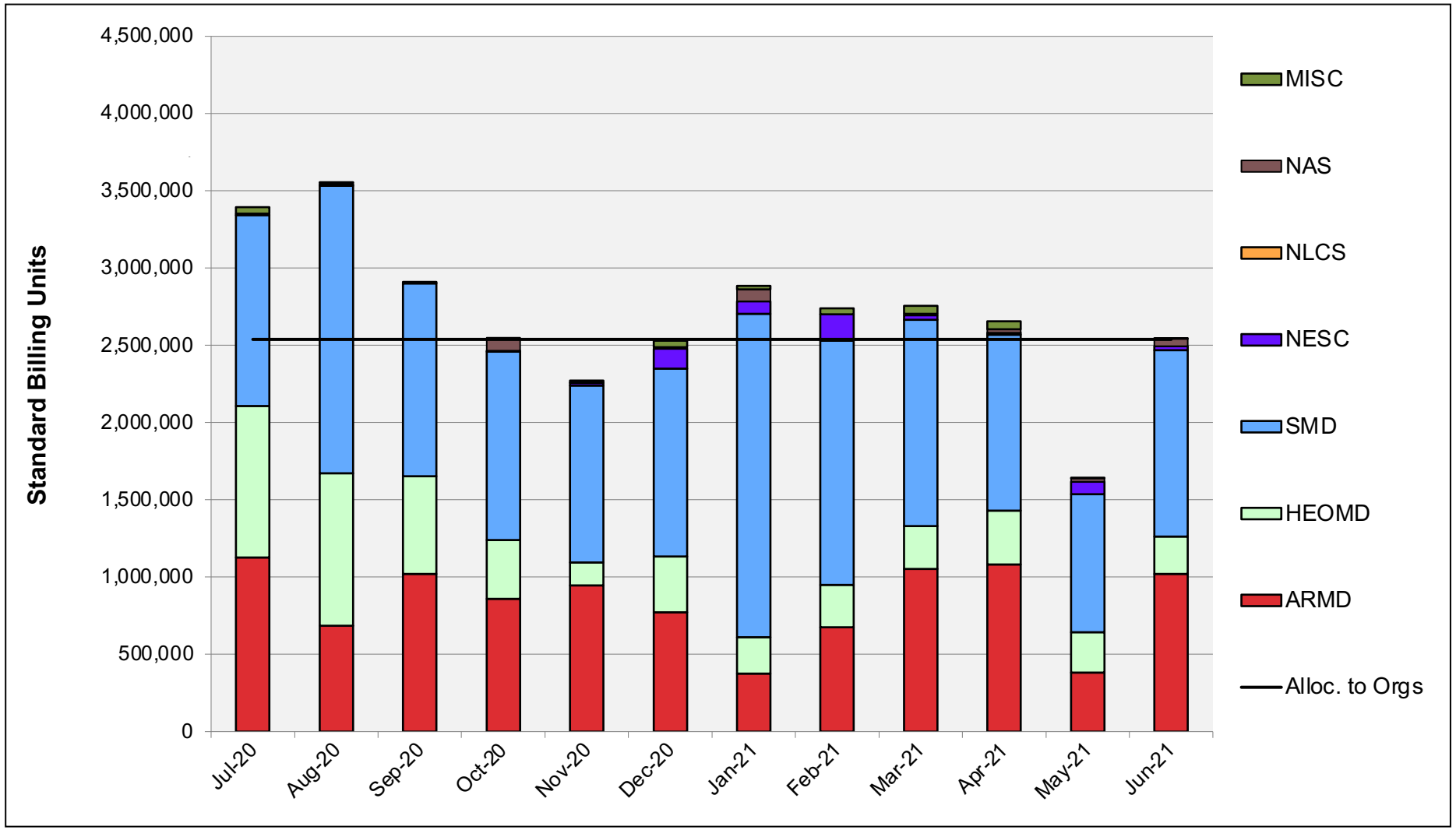

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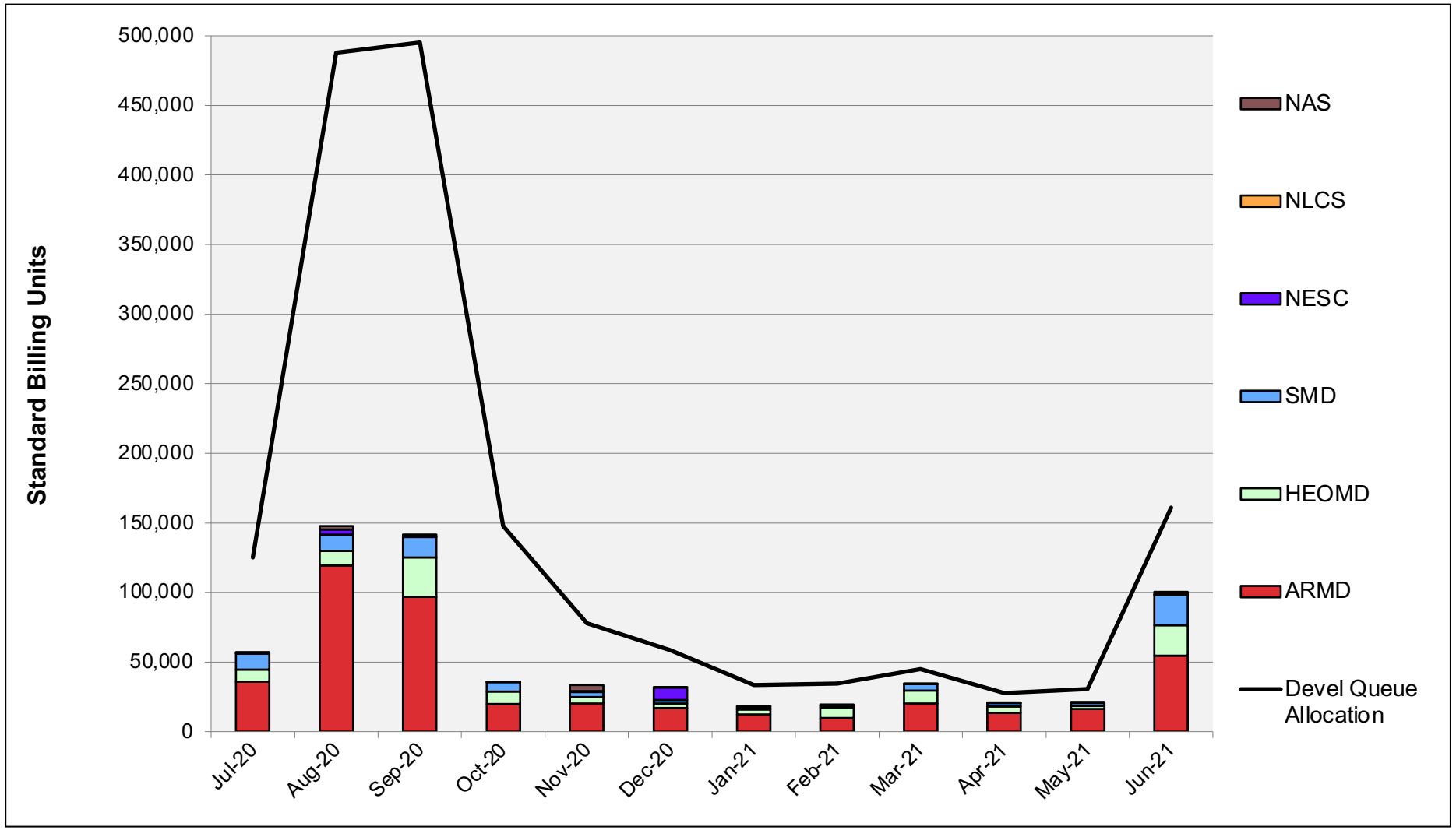
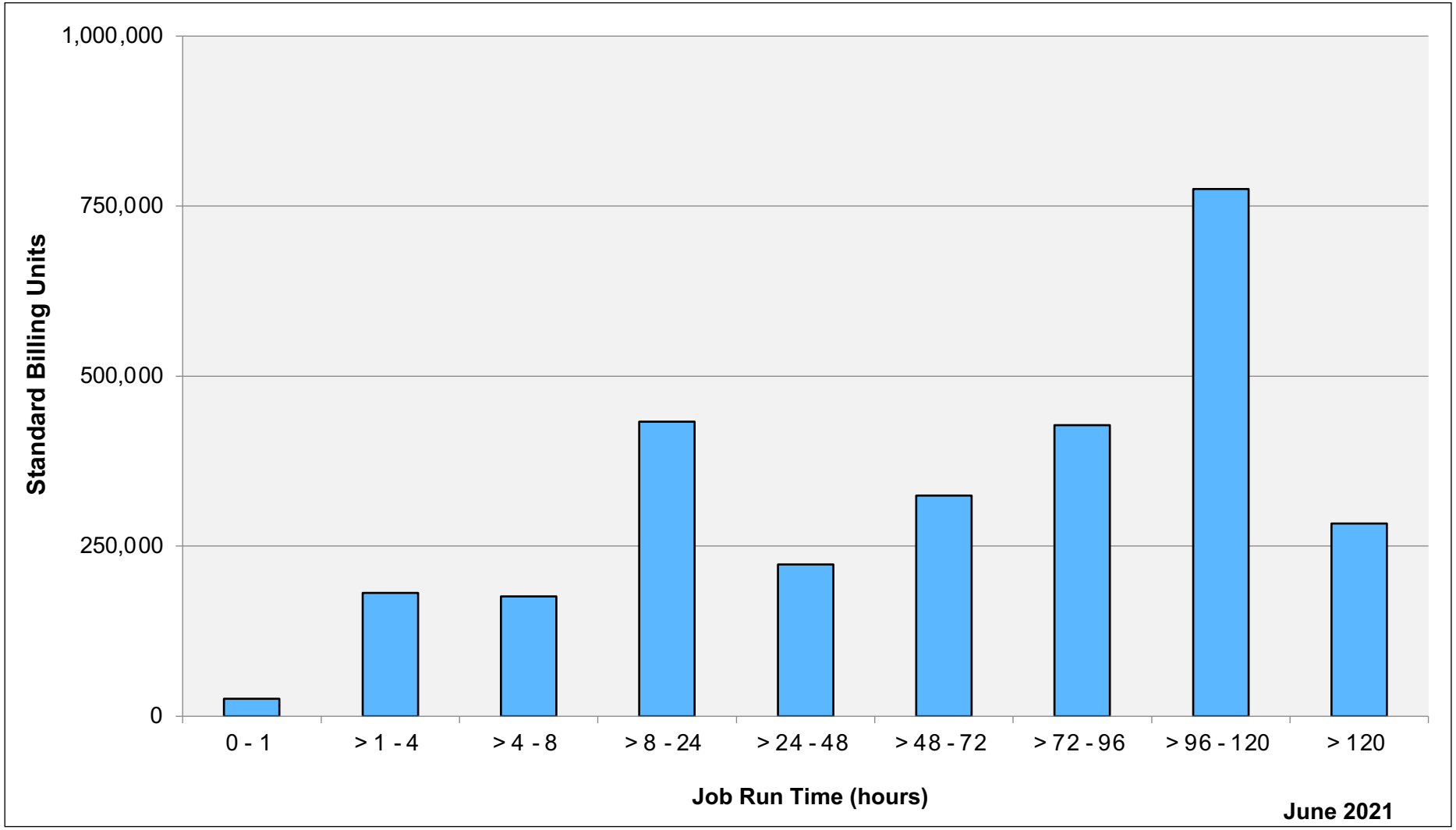
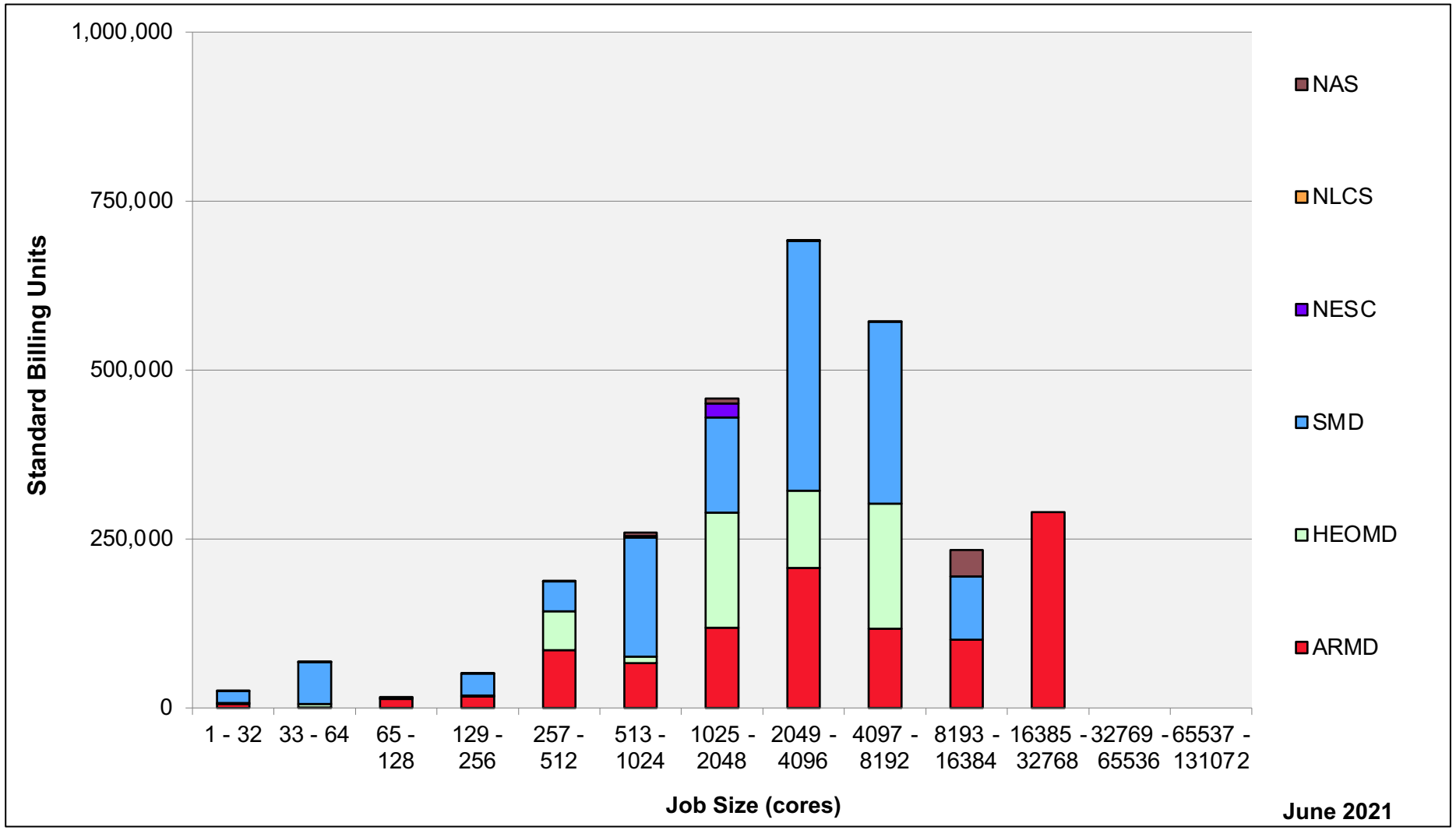


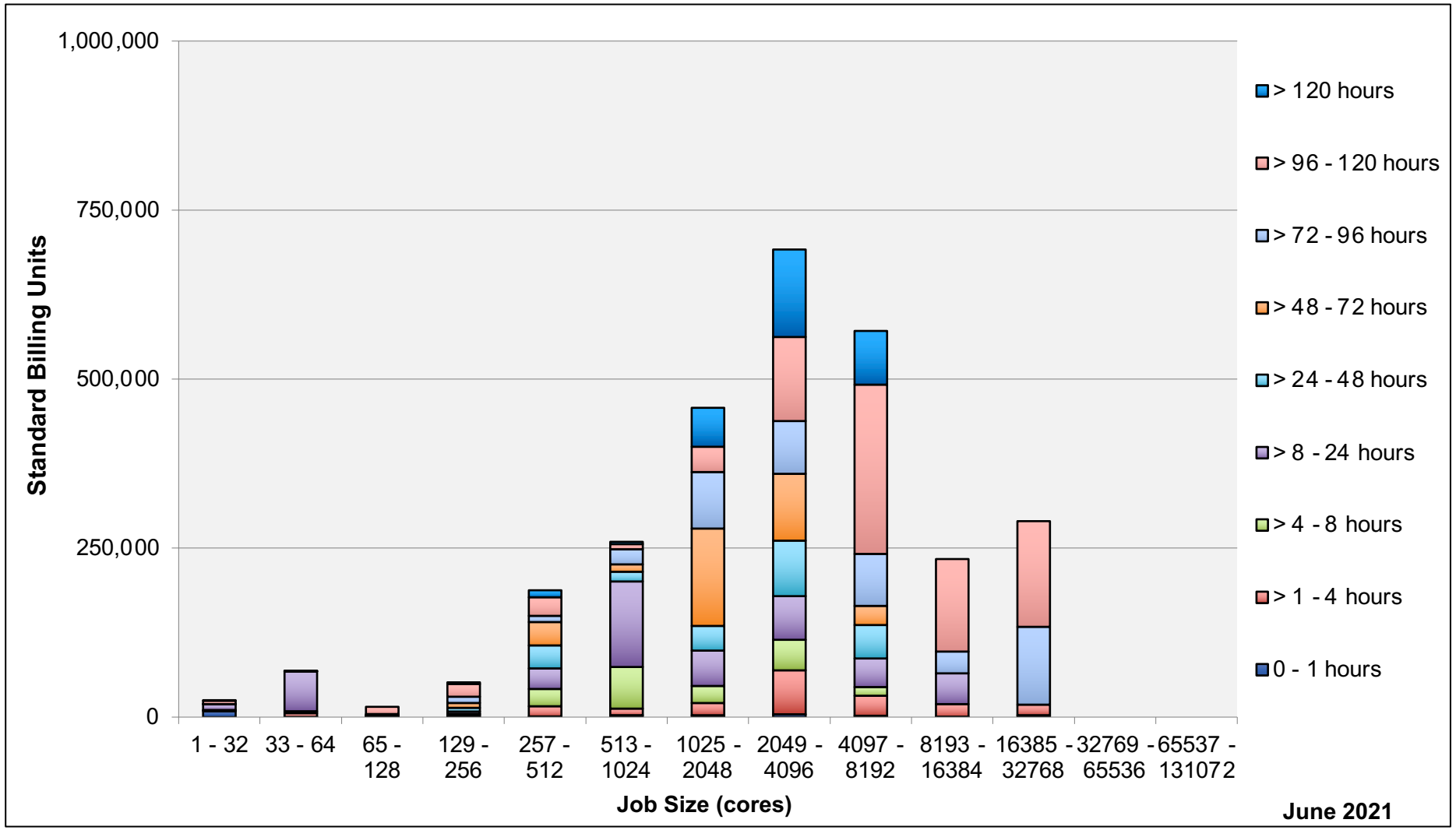
Electra: Monthly Utilization by Job Length



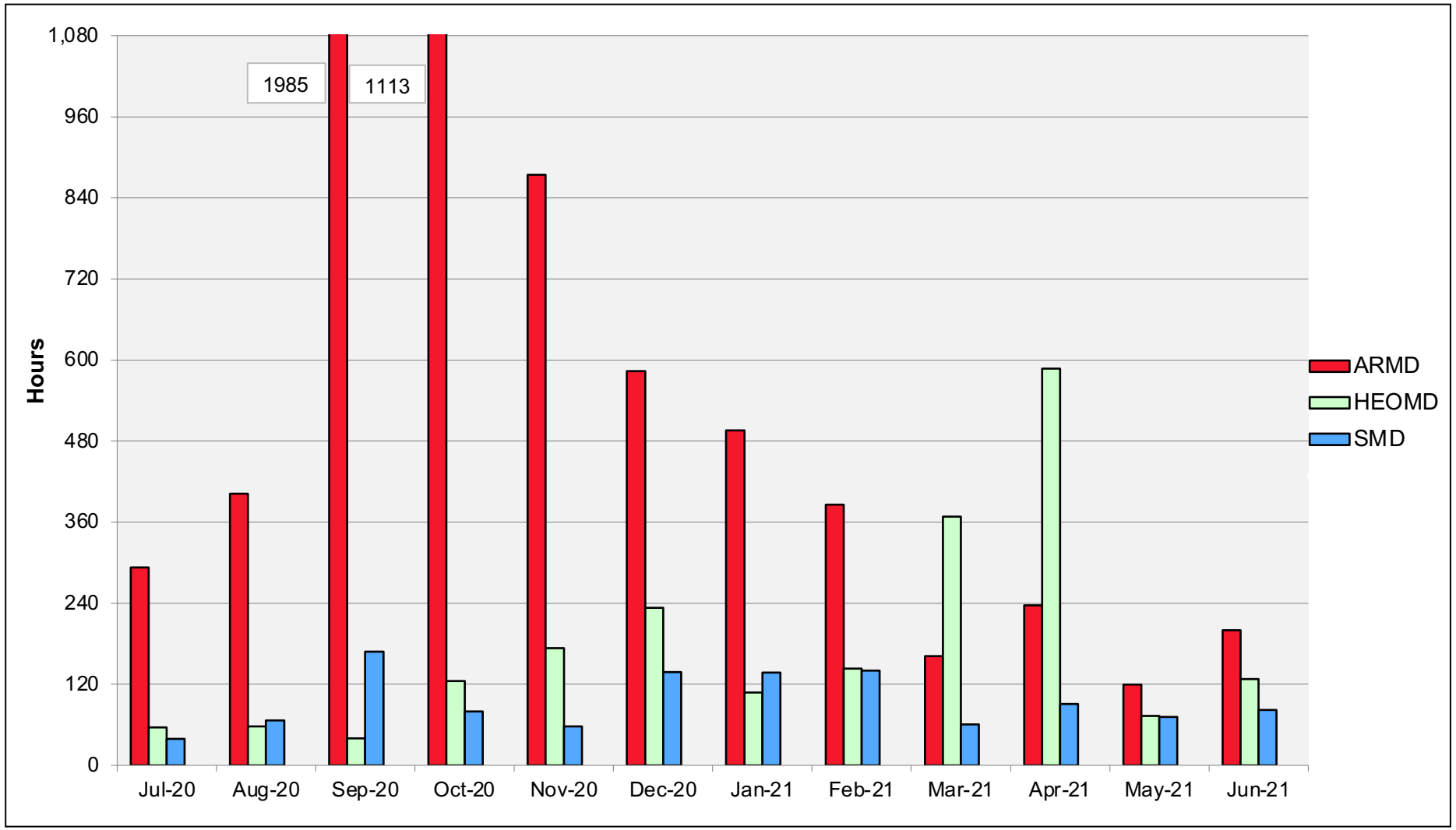
Electra: Monthly Utilization by Job Size



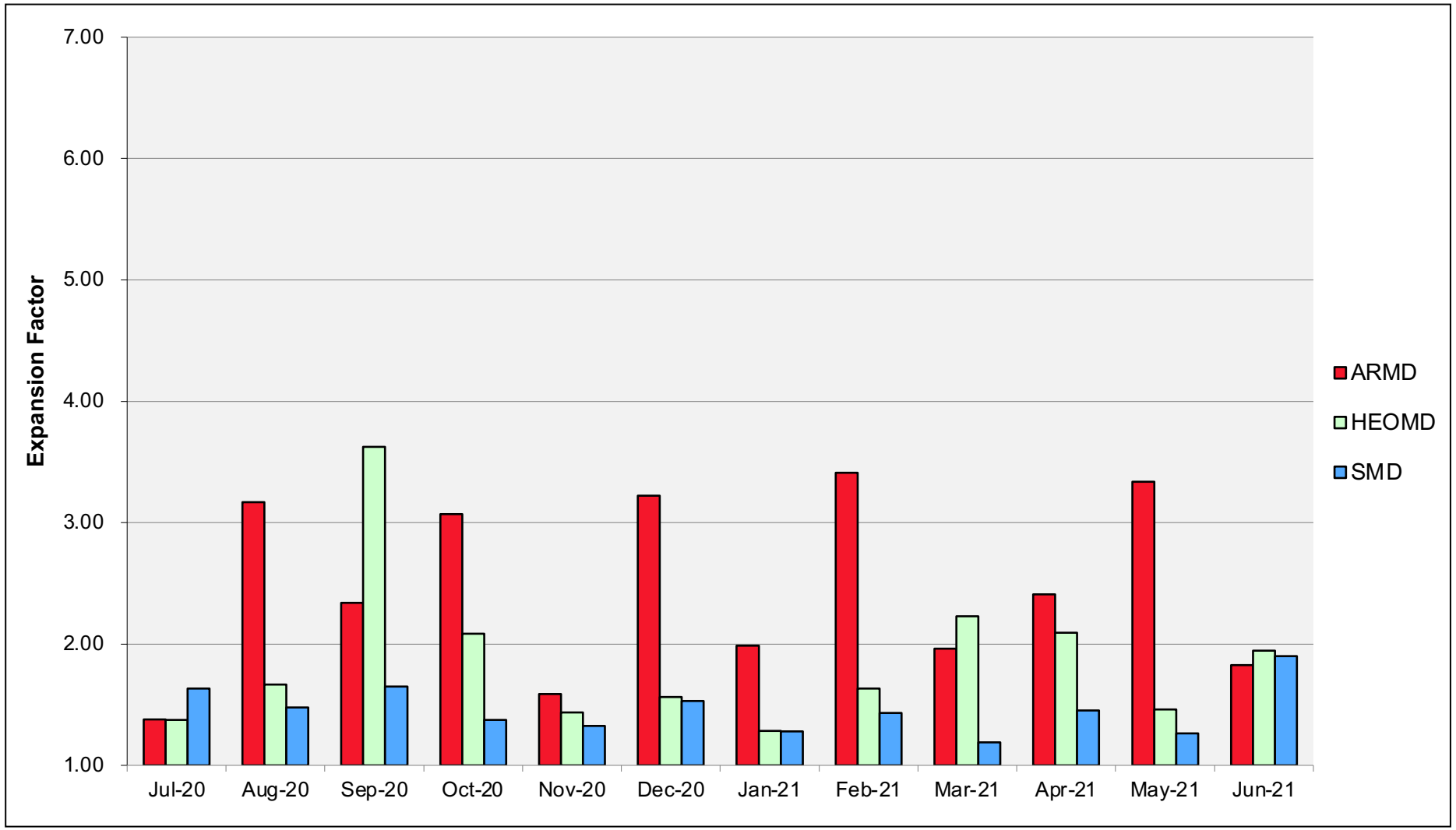
Electra: Monthly Utilization by Size and Length



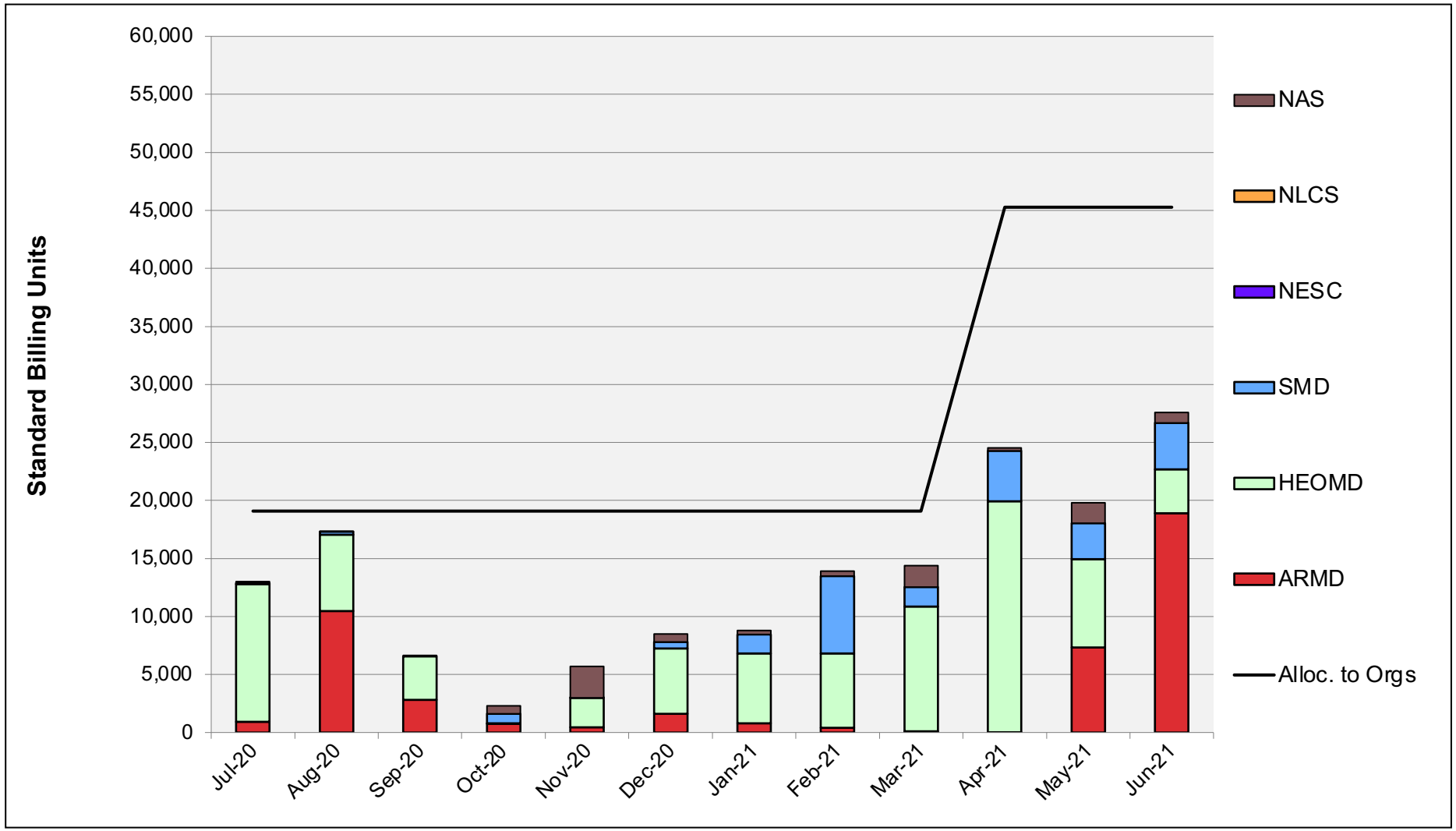
Electra: Average Time to Clear All Jobs



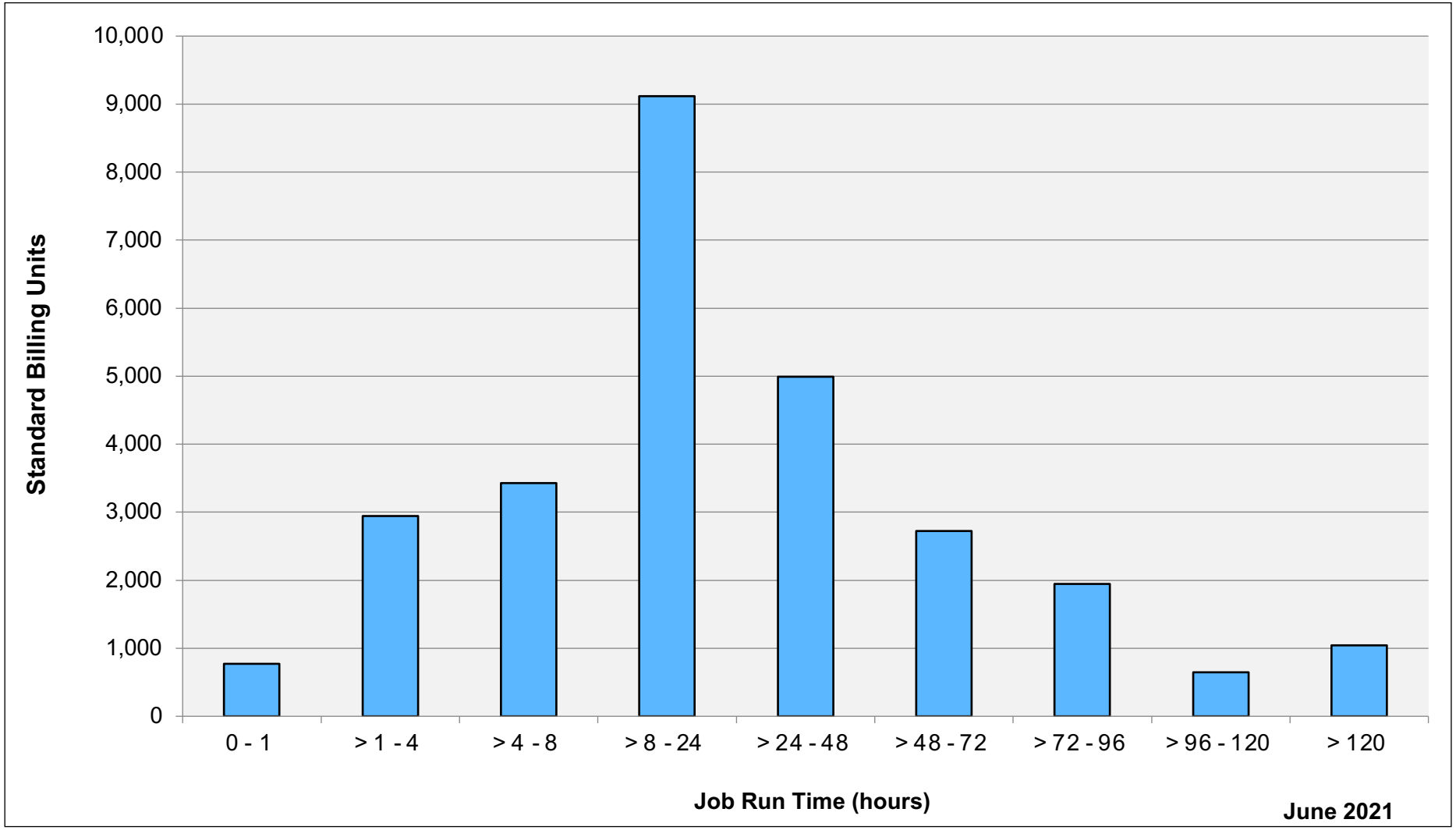
Electra: Average Expansion Factor



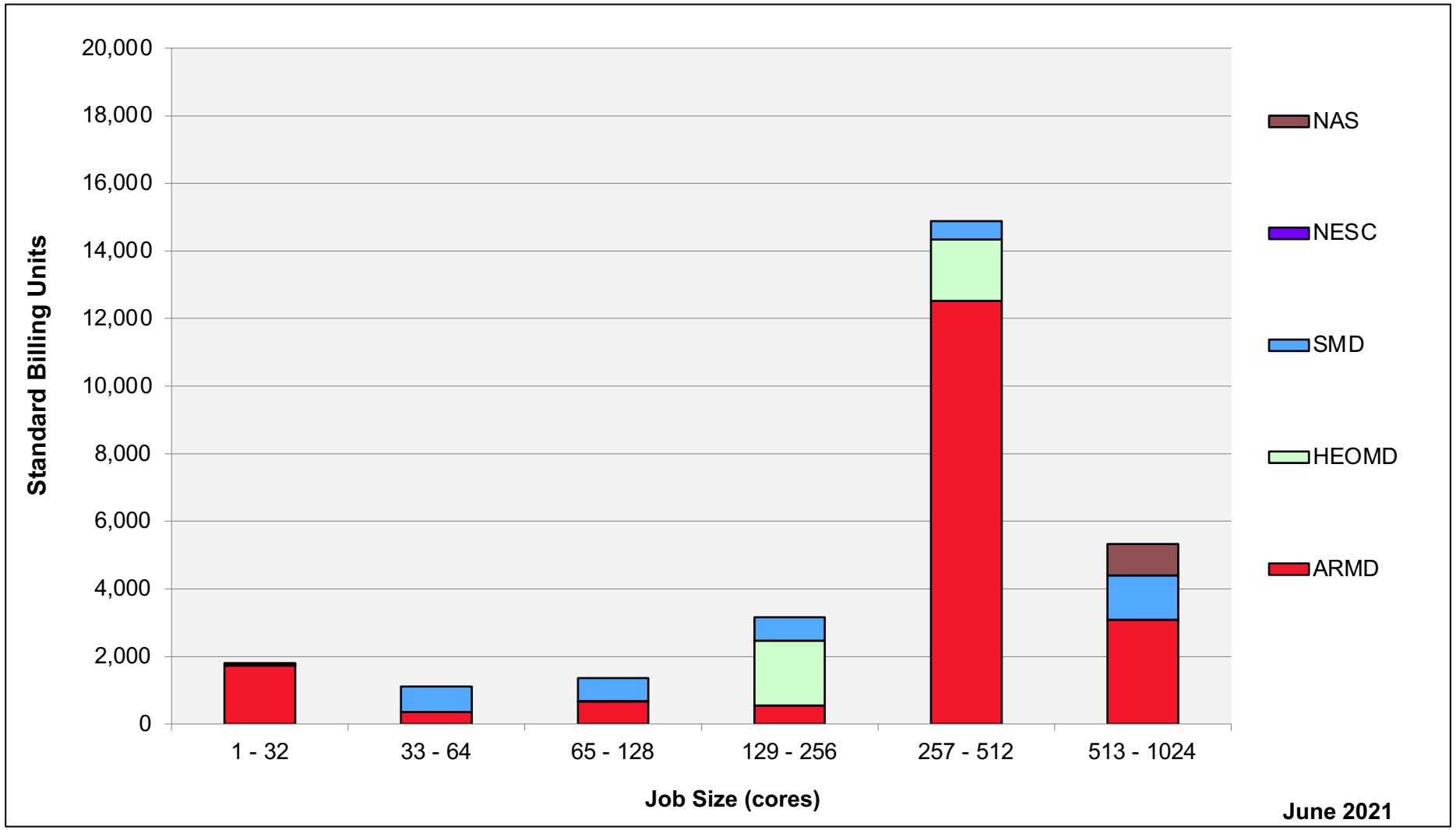
Endeavour: SBUs Reported, Normalized to 30-Day Month



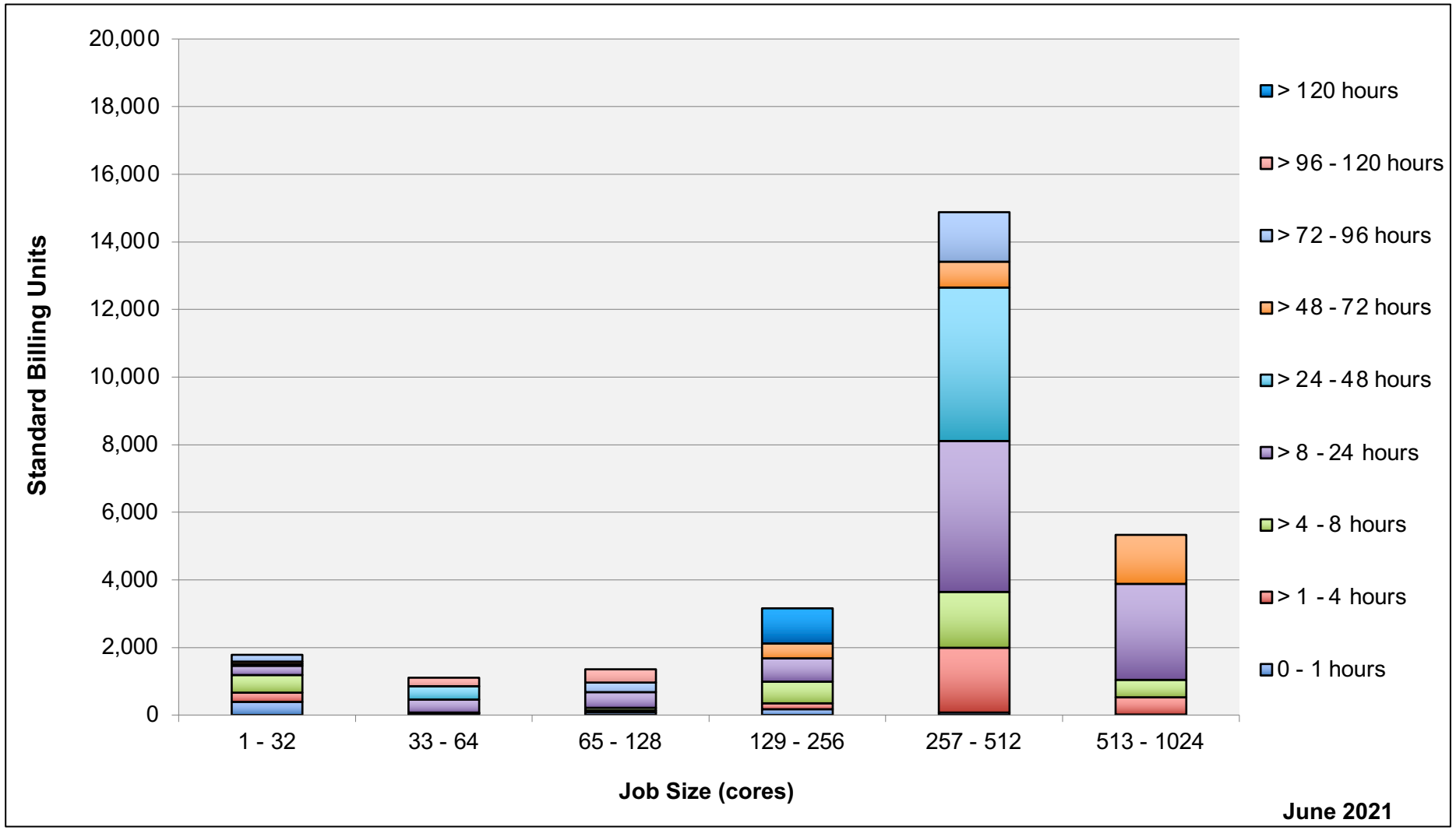
Endeavour: Monthly Utilization by Job Length



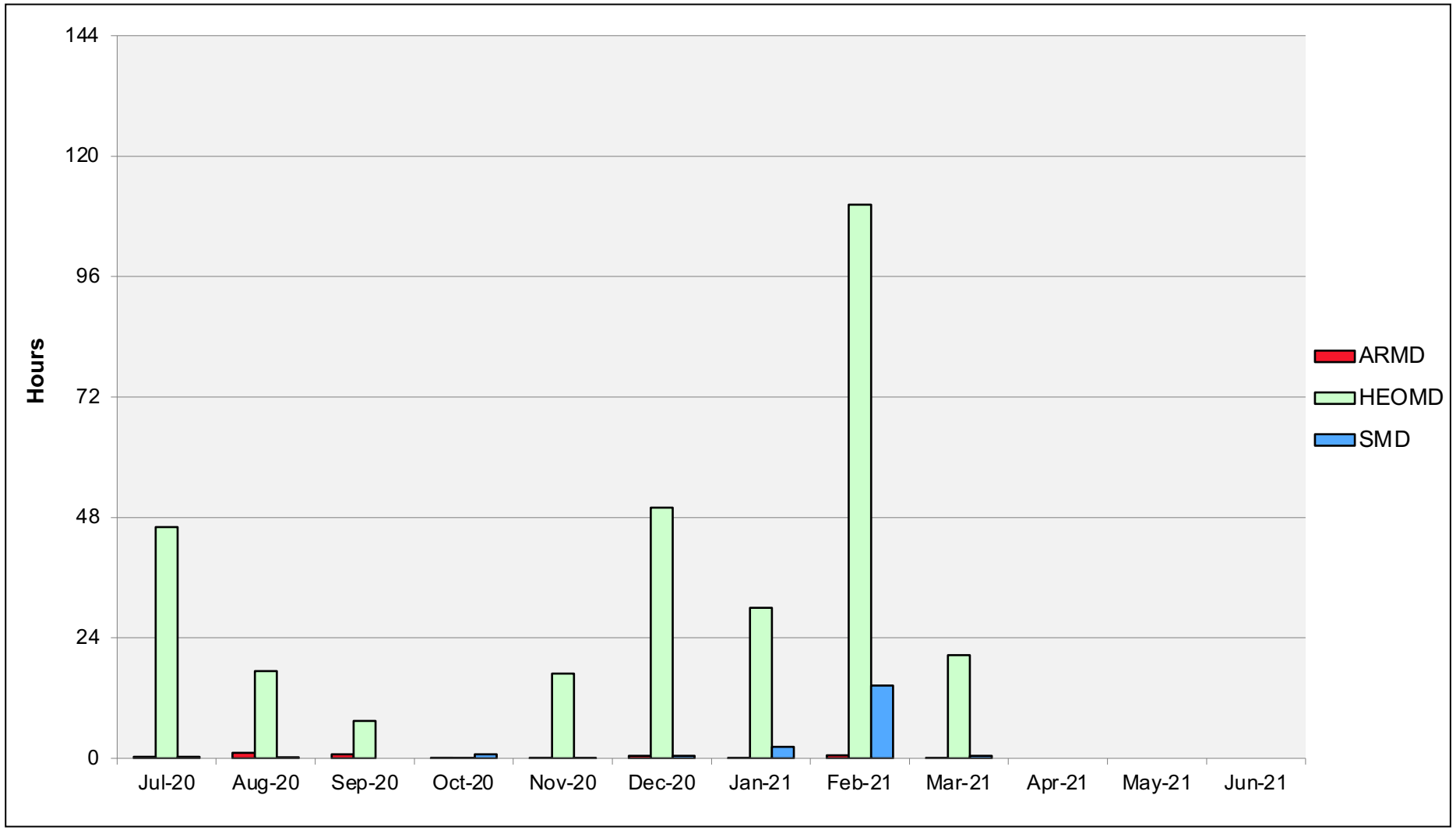
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor